The Structural Properties of (2, 6)-Fullerenes

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Abstract: A (2, 6)-fullerene \( F \) is a 2-connected cubic planar graph whose faces are only 2-length and 6-length. Furthermore, it consists of exactly three 2-length faces by Euler’s formula. The (2, 6)-fullerene comes from Došlić’s \((k, 6)\)-fullerene, a 2-connected 3-regular plane graph with only \(k\)-length faces and hexagons. Došlić showed that the \((k, 6)\)-fullerenes only exist for \( k = 2, 3, 4, \) or 5, and some of the structural properties of \((k, 6)\)-fullerene for \( k = 3, 4, \) or 5 were studied. The structural properties, such as connectivity, extendability, resonance, and anti-Kekulé number, are very useful for studying the number of perfect matchings in a graph, and thus for the study of the stability of the molecular graphs. In this paper, we study the properties of \((2, 6)\)-fullerene. We discover that the edge-connectivity of \((2, 6)\)-fullerenes is 2. Every \((2, 6)\)-fullerene is 1-extendable, but not 2-extendable (\( F \) is called \( n \)-extendable (\(|V(F)| \geq 2n + 2\)) if any matching of \( n \) edges is contained in a perfect matching of \( F \). \( F \) is said to be \( k \)-resonant (\( k \geq 1 \)) if the deleting of any \( i \) (\( 0 \leq i \leq k \)) disjoint even faces of \( F \) results in a graph with at least one perfect matching. We have that every \((2, 6)\)-fullerene is 1-resonant. An edge set, \( S \), of \( F \) is called an anti-Kekulé set if \( F - S \) is connected and has no perfect matchings, where \( F - S \) denotes the subgraph obtained by deleting all edges in \( S \) from \( F \). The anti-Kekulé number of \( F \), denoted by \( ak(F) \), is the cardinality of a smallest anti-Kekulé set of \( F \). We have that every \((2, 6)\)-fullerene \( F \) with \( |V(F)| > 6 \) has anti-Kekulé number 4. Further we mainly prove that there exists a \((2, 6)\)-fullerene \( F \) having \( f_6 \) hexagonal faces, where \( f_6 \) is related to the two parameters \( n \) and \( m \).

Keywords: (2, 6)-fullerene; edge-connectivity; anti-Kekulé number; resonance

1. Introduction

A (2, 6)-fullerene \( F \) is a 2-connected cubic planar graph whose faces are only 2-length and 6-length. The (2, 6)-fullerene comes from Došlić’s \((k, 6)\)-fullerene. A \((k, 6)\)-fullerene is a 2-connected cubic planar graph whose faces are only \( k \)-length and 6-length. Došlić showed that all \((k, 6)\)-fullerenes only exist for \( k = 2, 3, 4, \) or 5, and are 1-extendable [1]. A \((5, 6)\)-fullerene is the usual fullerene as the molecular graph of a sphere carbon fullerene. A \((4, 6)\)-fullerene is the molecular graph of a boron–nitrogen fullerene. The structural properties, such as connectivity, extendability, resonance, and anti-Kekulé number, are very useful for studying the number of perfect matchings in a graph [2,3]. And the number of perfect matchings is closely related to the stability of molecular graphs [4–8]. Therefore, many articles have studied the structural properties of graphs in both mathematics and chemistry [9–11]. In 2002, Došlić showed that fullerene graphs are bicritical and 2-extendable [9,12]. At the same time, he showed that every fullerene graph is cyclically 5-edge-connected [1]. In 2008, Kardoš characterized the cyclic edge-cuts of fullerene graphs by means of three operations [13]. For the resonance of fullerene graphs, in 2009, Ye et al. proved that every fullerene graph is 1-resonant and all leapfrog fullerene graphs are 2-resonant [14]. Later, Kaiser showed that the IPR fullerene graphs are also 2-resonant [15]. In 2010, Zhang et al. showed that boron–nitrogen fullerene graphs are bipartite, 3-connected, and 1-extendable [16]. They also proved that every boron–nitrogen fullerene is 2-resonant [16]. In 2011, Jiang et al. proved that boron–nitrogen fullerene graphs...
have the forcing number at least two [17]. A (3, 6)-fullerene is 1-extendable, and has the connectivity 2 or 3 [18]. In 2012, Yang et al. showed that each hexagon of a (3, 6)-fullerene with connectivity 2 is not resonant, and each hexagon of a (3, 6)-fullerene with connectivity 3 is resonant except for one graph [19]. This paper is mainly concerned with the structural properties of (2, 6)-fullerenes.

A (2, 6)-fullerene $F$ is a cubic planar graph such that every face is either 2-length or 6-length. A graph with two vertices and $n$ parallel edges joining them is denoted by $n \times K_2$. The smallest (2, 6)-fullerene is $3 \times K_2$. A plane graph is a graph that can be embedded in the plane such that its edges intersect only at their ends. Any such embedding divides the plane into connected regions called faces. Two different faces, $f_1, f_2$, are adjacent if their boundaries have an edge in common. A face is said to be incident with the vertices and edges in its boundary, and vice versa. An edge is said to be incident with the ends of the edge, and vice versa. Two vertices that are incident with a common edge are adjacent, and two distinct adjacent vertices are neighbors. If $S$ is a set of vertices in a graph, $F$, the set of all neighbors of the vertices in $S$ is denoted by $N(S)$, and $|N(S)|$ denotes the number of neighbors of $S$.

Let $F$ be a (2, 6)-fullerene with vertex-set $V(F)$ and edge-set $E(F)$. We denote the number of vertices and edges in $F$ by $|V(F)|$ and $|E(F)|$. For $H \subseteq F$, we let $F - H$ be the subgraph of $F$ obtained from $F$ by removing the elements in $H$. A matching of $F$ is a set of disjoint edges, $M$, of $F$. A perfect matching of $F$ is a matching $M$ that covers all vertices of $F$. A perfect matching of a graph coincides with a Kekulé structure of some molecular graph in organic chemistry. A set, $\mathcal{H}$, of disjoint even faces of a graph, $F$, is a resonant pattern if $F$ has a perfect matching $M$ such that the boundary of each face in $\mathcal{H}$ is an $M$-alternating cycle. $F$ is said to be $k$-resonant ($k \geq 1$) if any $i$ ($0 \leq i \leq k$) disjoint even faces of $F$ form a resonant pattern. Moreover, $F$ is called $n$-extendable ($|V(F)| \geq 2n + 2$) if any matching of $n$ edges is contained in a perfect matching of $F$. $F$ is bicritical if $F$ contains an edge and $F - u - v$ contains a perfect matching, for every pair of distinct vertices $u, v \in V(F)$. In this paper, we show that every (2, 6)-fullerene is 1-extendable, 1-resonant but not 2-extendable, bicritical.

The anti-Kekulé set of a (2, 6)-fullerene $F$ with perfect matchings is an edge set, $S \subseteq E(F)$, such that $F - S$ is connected and has no perfect matchings. The anti-Kekulé number of $F$, denoted by $ak(F)$, is the cardinality of a smallest anti-Kekulé set of $F$. It is NP-complete to find the smallest anti-Kekulé set of a graph. Moreover, it has been shown that the anti-Kekulé set of a graph significantly affects the whole molecule structure by the valence bond theory. We know the (5, 6), (4, 6), and (3, 6)-fullerenes have the anti-Kekulé numbers 4, 4, and 3, respectively. In this paper, We show that every (2, 6)-fullerene $F$ has the anti-Kekulé number 4, with $|V(F)| > 6$.

2. Main Results

An edge-cut of $F$ is a subset of edges $E' \subseteq E(F)$ such that $F - E'$ is disconnected. An $k$-edge-cut is an edge-cut with $k$ edges. The edge-connectivity of $F$, denoted by $\kappa'(F)$, is equal to the minimum cardinality of edge-cuts. $F$ is $k$-edge-connected if $F$ cannot be separated into at least two components by removing fewer than $k$ edges.

Lemma 1. The (2, 6)-fullerene $F$ has edge-connectivity 2, where $|V(F)| > 2$.

Proof. Since every edge of $F$ is incident with a 2-length face or a 6-length face, there is no cut edge in $F$. Therefore, $F$ is 2-edge-connected. For one 2-length face, $C$, in $F$, we denote it by $C = xyy$. Then either $F \cong 3 \times K_2$ or the two edges incident with $x$ and $y$, respectively, other than $xy$ form an 2-edge-cut of $F$. Therefore, $\kappa'(F) = 2$, where $|V(F)| > 2$. \hfill $\square$

We say an edge, $e$, is incident to a subgraph, $H$, if $|V(e) \cap V(H)| = 1$.

Lemma 2. Every 2-edge-cut of a (2, 6)-fullerene isolates a 2-length face.
Proof. Let $F$ be a (2,6)-fullerene. If $|V(F)| = 2$, then $F \cong 3 \times K_2$, and the conclusion holds as $F$ has no 2-edge-cut. So, next we suppose $|V(F)| > 2$. By Lemma 1, $F$ has an 2-edge-cut. Let $E = \{e_1, e_2\}$ be an 2-edge-cut whose deletion separates $F$ into two components, $F'$ and $F''$. Then $E$ is a matching of $F$, as $F$ is 3-regular and has edge-connectivity 2. Suppose every edge, $e_i$, has one endpoint, say $x_i$, on $F'$, and the other endpoint, say $y_i$, on $F''$, $i = 1, 2$. Suppose the outer face of $F''$ is exactly the outer face of $F$, thus $F'$ lies in some inner face of $F''$. Then, there are two hexagons, denoted by $f_1$ and $f_2$, such that both $f_1$ and $f_2$ are incident with $x_1, x_2, y_1$, and $y_2$. If one of $F'$ and $F''$ contains a cut edge, without losing generality, assume that $F'$ contains a cut edge, $e = uv$, then $F' - e$ has two connected components, say $F_1$ and $F_2$. Then, both $e_1$ and $e_2$ cannot be incident to the same component $F_i$ ($i = 1, 2$), otherwise there exists a cut edge, $e$, in $F$, which is a contradiction. Then, $V(f_1) = \{u, v, x_1, y_1, x_2, y_2\}$, $V(f_2) = \{u, v, x_1, y_1, x_2, y_2\}$. That is, all of $F_1$, $F_2$, and $F''$ are 2-length faces and we obtain a (2,6)-fullerene with six vertices, and thus the conclusion holds. If both $F'$ and $F''$ contain cut edges, then there is a face with length more than 6, which is a contradiction. If neither $F'$ nor $F''$ has a cut edge, then $F'$ and $F''$ are 2-edge-connected, and in each of them there is only one face that is not 2-length or 6-length, and we denote these two boundaries of the exceptional faces by $C'$ and $C''$, respectively. Let $v'$, $e'$, and $f'$ be the number of vertices, edges, and faces in $F'$, respectively. Let $l'$ be the length of $C'$, and $f'_2$ and $f'_6$ be the number of 2-length faces and 6-length faces in $F'$, respectively. By Euler’s formula and the structure of $F'$, it follows that

$$\begin{cases} 3v' = 2e' + 2 \\ v' - e' + f'_2 + f'_6 = 1 \\ 2f'_2 + 6f'_6 + l' = 2e'. \end{cases}$$

(1)

By (1), we obtain that

$$l' = 4f'_2 - 2.$$  

(2)

Since $F$ has no face with length more than 6, each of the two faces, $f_1$ and $f_2$, has at most two additional vertices on $C'$. Hence, $2 \leq l' \leq 6$. By (2), we can obtain $1 \leq f'_2 \leq 2$. If $f'_2 = 1$, we have $l' = 2$, which means that $F'$ is a 2-length face, and thus the conclusion holds. If $f'_2 = 2$, then $l' = 6$ and there are no additional vertices on $C''$, which implies that $F''$ is a 2-length face, and thus the conclusion holds. Therefore, every 2-edge-cut of a (2,6)-fullerene isolates a 2-length face. $\square$

In [1], Došlić proved that the $(k,6)$-fullerene is 1-extendable for $k = 3, 4$, and 5. In fact, we may observe that the conclusions remain valid for $k = 2$.

Lemma 3 ([1]). Let $F$ be a (2,6)-fullerene graph. Then $F$ is 1-extendable.

The resonance of faces of a plane bipartite graph is closely related to a 1-extendable property. It was revealed that every face (including the infinite one) of a plane bipartite graph $G$ is resonant if and only if $G$ is 1-extendable [20]. Combing with Lemma 3, we know that every (2,6)-fullerene is 1-resonant.

Corollary 1. Every (2,6)-fullerene is 1-resonant.

Moreover, we know no (2,6)-fullerene is 2-extendable.

Theorem 1. No (2,6)-fullerene is 2-extendable.

Proof. Let $F$ be a (2,6)-fullerene graph. Let $f$ be a 2-length face of $F$ with the boundary $v_1v_2v_3$. By the definition of extendability, we know that $|V(F)| \geq 4$. Then, there exist two vertices, $u_1$ and $u_2$, of $F$, which are different from $v_1$ and $v_2$ such that $u_1v_1 \in E(F)$ and $u_2v_2 \in E(F)$. Since the four vertices, $u_1, u_2, v_1$, and $v_2$, must be contained in the same hexagon of $F$, there is a vertex, $u_3 \neq u_1, u_3 \neq v_2$, of $F$ such that $u_2u_3 \in E(F)$. Obviously,
\(u_1v_1, u_2u_3\) is a matching and cannot be contained in a perfect matching of \(F\). Thus, no \((2,6)\)-fullerene is 2-extendable. \(\square\)

Similarly, we can show no \((2,6)\)-fullerene is bicritical.

**Theorem 2.** No \((2,6)\)-fullerene is bicritical.

**Proof.** Let \(F\) be a \((2,6)\)-fullerene graph, and \(f\) be a 2-length face of \(F\) with the boundary \(v_1v_2v_1\). If \(F \cong 3 \times K_2\), then \(F - v_1 - v_2\) has no perfect matchings. If \(F \not\cong 3 \times K_2\), then there exists a vertex, \(u\), of \(F\), which is different from \(v_2\) such that \(uv_1 \in E(F)\). Then, \(F - u - v_2\) has a single vertex, \(v_1\), as a component. So, \(F - u - v_2\) has no perfect matchings. That is, \(F\) is not bicritical. \(\square\)

**Theorem 3 (Tutte’s Theorem [21]).** A graph \(G\) has a perfect matching if and only if \(c_o(G - U) \leq |U|\) for any \(U \subseteq V(G)\), where \(c_o(G - U)\) is the number of odd components of \(G - U\).

**Theorem 4 (Hall’s Theorem [21]).** Let \(F\) be a bipartite graph with bipartition \(W\) and \(B\). Then \(F\) has a perfect matching if and only if \(|W| = |B|\) and for any \(U \subseteq W\), \(|N(U)| \geq |U|\) holds.

For the connected cubic simple bipartite graph, we know its anti-Kekulé number is 4 [22].

**Theorem 5 ([22]).** If \(G\) is a connected cubic simple bipartite graph, then \(ak(F) = 4\).

The above result can be used to determine the anti-Kekulé numbers of some interesting graphs, such as \((4,6)\)-fullerenes [22], toroidal fullerenes [22], etc. Theorem 5 is also valid for \((2,6)\)-fullerene when \(|V(F)| > 6\).

**Theorem 6.** Let \(F\) be a \((2,6)\)-fullerene graph with \(|V(F)| > 6\). Then \(ak(F) = 4\).

**Proof.** Let \(F\) be a \((2,6)\)-fullerene. For any vertex, \(u\), in \(F\), if \(|N(u)| = 1\), then \(F \cong 3 \times K_2\) (see Figure 1a the graph \(3 \times K_2\)). For any vertex, \(u\), in \(F\), if \(|N(u)| = 2\), then \(F \cong F_6\) (see Figure 1b the graph \(F_6\)). We can easily see that both \(3 \times K_2\) and \(F_6\) cannot exist the anti-Kekulé set. On the other hand, if we let \(n\) and \(f_6\) be the number of vertices and the hexagons of \(F\), respectively, then, by Euler’s formula and the formula of degree sum, we can obtain \(n = 2f_6 + 2\). Thus, if \(f_6 = 0\), then \(n = 2\) and \(F \cong 3 \times K_2\). If \(f_6 = 1\), then \(n = 4\), which is impossible as every hexagonal face must contain six vertices. If \(f_6 = 2\), then \(n = 6\) and \(F \cong F_6\) (see Figure 1b the graph \(F_6\)). Therefore, when \(|V(F)| \leq 6\), there is no anti-Kekulé set in \(F\).

\[\text{(a) } 3 \times K_2 \quad \text{(b) } F_6\]

**Figure 1.** The \((2,6)\)-fullerenes \(3 \times K_2\) (a), \(F_6\) (b).

Next, we discuss the anti-Kekulé number of \(F\) with \(|V(F)| > 6\). Then, there is a vertex, \(u\), in \(F\) and \(|N(u)| = 3\). Let \(x, y, z\) be the three neighbors of \(u\). Let \(e_1\) and \(e_2\) be two edges incident with \(x\) other than \(ux\), and let \(e_3\) and \(e_4\) be two edges incident with \(y\) other than \(uy\). Since every face of \(F\) is 2-length or 6-length and \(F\) is 2-edge-connected, the four edges \(e_1, e_2, e_3, e_4\) are pairwise different. We claim that \(\{e_1, e_2, e_3, e_4\}\) is an anti-Kekulé set. It is obvious that \(F - \{e_1, e_2, e_3, e_4\}\) has no perfect matchings as the two vertices, \(x, y\), cannot be contained in the same perfect matching. If \(F - \{e_1, e_2, e_3, e_4\}\) is no connected,
then we obtain a cut edge, $uz$, in $F$, contradicting Lemma 1. Then, we find an anti-Kekulé set of size 4, and so $ak(F) \leq 4$.

In the following, we show $ak(F) \geq 3$. Let $A$ be an anti-Kekulé set of size $ak(F)$. Then $F' = F - A$ is connected and has no perfect matchings. According to Theorem 3, there exists $S \subseteq V(F')$ such that $c_0(F' - S) > |S|$. If we choose such an $S$ with the maximum size, then $F' - S$ has no even components. On the contrary, suppose that $F' - S$ has an even component, $H$. For any vertex $v \in V(H)$, $c_0(H - v) \geq 1$. Let $S' = S \cup \{v\}$, then $c_0(F' - S') \geq c_0(F' - S) + 1 > |S| + 1 = |S'|$, which is a contradiction to the choice of $S$.

Since $|V(F')|$ is even, then $c_0(F' - S) \geq |S| + 2$ by parity. For any edge $e \in A$, adding $e$ to $F' - S$ will connect at most two odd components, then $c_0(F' + e - S) \geq c_0(F' - S) - 2$.

Since $A$ is the smallest anti-Kekulé set of $F$, then $F' + e$ has a perfect matching for any edge $e \in A$. Hence, by Theorem 3, for the above subset $S$, $c_0(F' + e - S) \leq |S|$. Therefore, $|S| \geq c_0(F' + e - S) \geq c_0(F' - S) - 2 \geq |S|$. We obtain $c_0(F' - S) = |S| + 2$, and the edge, $e$, connects exactly two components of $F' - S$.

Let $F_i$ be the odd components of $F' - S$, where $1 \leq i \leq |S| + 2$. For $F_i \subseteq F$, let $d(F_i)$ denote the number of the set of edges with one end in $F_i$ and the other end in $F - F_i$. Denote the number of edges between $S$ and the odd components by $N$. Since $F$ is cubic, $S$ sends out at most $3|S|$ to $N$. In addition, $\sum_{i=1}^{\lfloor |S|/2 \rfloor} d(F_i)$ sends out exactly $\sum_{i=1}^{\lfloor |S|/2 \rfloor} d(F_i) - 2ak(F)$ edges to $N$. Hence

$$N = \sum_{i=1}^{\lfloor |S|/2 \rfloor} d(F_i) - 2ak(F) \leq 3|S|.$$ (3)

Because $F$ is 2-edge-connected, $d(F_i) \geq 2$ for every $i$. On the other hand, $d(F_i) = 3|V(F_i)| - 2|E(F_i)|$, which implies that $d(F_i)$ and $|V(F_i)|$ are of the same parity. Every $F_i$ sends odd number edges, hence $d(F_i) \geq 3$. Substituting it into (3), we have

$$3(|S| + 2) - 2ak(F) \leq \sum_{i=1}^{\lfloor |S|/2 \rfloor} d(F_i) - 2ak(F) \leq 3|S|,$$

the above inequality gives $ak(F) \geq 3$.

We find that the anti-Kekulé number of $F$ is either 3 or 4. Suppose, on the contrary, that $ak(F) = 3$. Then there exists an anti-Kekulé set, $A = \{e_1, e_2, e_3\}$, of cardinality three in $F$, such that $F - A$ is connected and has no perfect matchings. Assume $B$ and $C$ be the bipartition of $F$. By Hall’s theorem, there exists $U \subseteq W$ such that

$$|N_{F-A}(U)| \leq |U| - 1$$ (4)

where $N_{F-A}(U)$ means $N(U)$ in $F - A$. Moreover, for $e_i \in A$, since $A$ is the smallest anti-Kekulé set, $F - A + e_i$ has a perfect matching. Immediately, by Theorem 4, for the above subset $U$,

$$|U| \leq |N_{F-A+e_i}(U)|$$ (5)

for $i = 1, 2,$ and $3$, where $N_{F-A+e_i}(U)$ means $N(U)$ in $F - A + e_i$. In addition, the neighbors of $U$ will be increased by at most one if we add an edge, $e_i$, to $F - A$. Hence

$$|N_{F-A+e_i}(U)| \leq |N_{F-A}(U)| + 1.$$ (6)

Combining inequalities (4)–(6), we have $|U| = |N_{F-A}(U)| + 1$, and $e_i$ is incident with the vertices of $U$ and $B - N_{F-A+e_i}(U)$ in $F - A + e_i$. Thus, the edges going out from $U \subseteq V(F)$ either go into $A$ or go into the edges going out from $N_{F-A}(U)$. Then, the number of edges between $U$ and $N_{F-A}(U)$ is $3|U| - 3$. Since $|N_{F-A}(U)| = |U| - 1$, $3|N_{F-A}(U)| = 3(|N_{F-A}(U)| + 1) - 3 = 3|U| - 3$, that is, there is no edge between $N_{F-A}(U)$ and $W - U$ in $F - A$. As a result, $A$ is an edge-cut, which is a contradiction to the definition of an anti-Kekulé set.
In [23], Grünbaum and Motzkin showed that (5,6)-fullerene and (4,6)-fullerene having \( n \) hexagonal faces exist for every non-negative integer, \( n \), satisfying \( n \neq 1 \), and gave a similar result for (3,6)-fullerene. Therefore, we consider whether (2,6)-fullerene having \( n \) hexagonal faces also exists for any \( n \). We tried to give a positive answer to this question, but we found that the conclusion seems quite elusive. Therefore, in this part, we mainly prove that there exists a (2,6)-fullerene \( F \) having \( f_F \) hexagonal faces, where \( f_F \) is related to the two parameters \( n \) and \( m \).

Let \( F \) be a (2,6)-fullerene. A fragment, \( H \), of \( F \) is a subgraph of \( F \) consisting of a cycle together with its interior and every inner face of \( H \) is also a face of \( F \). We define \( \partial(H) \) as the boundary of the exterior face of \( H \). A face, \( f \), of \( F \) is a neighboring face of \( H \) if \( f \) is not a face of \( H \) and \( f \) has at least one edge in common with \( H \). A path of length \( k \) (the number of edges) is called a \( k \)-path. Denote by \( f_H \) the number of hexagons of \( H \).

**Proposition 1.** In all the (2,6)-fullerenes, there exists a fragment, say \( G_n \), such that \( f_{G_n} = n^2 + n \), \( n \in \mathbb{Z} \).

**Proof.** Let \( G_0 \) be a 2-length face and \( f_{11} \) and \( f_{12} \) be two neighboring faces of \( G_0 \) (see Figure 2a). Then \( f_{G_0} = 0 \). Suppose that \( f_{11} \) and \( f_{12} \) are hexagons. Set \( G_1 = G_0 \cup \{f_{11}, f_{12}\} \), suppose both \( f_{11} \) and \( f_{12} \) are inner faces of \( G_1 \), and let \( f_{21}, f_{22}, f_{23}, \) and \( f_{24} \) be four neighboring faces of \( G_1 \) along the clockwise direction, such that \( f_{21} \) is incident with the two consecutive 2-degree vertices on \( \partial(G_1) \) (see Figure 2b). Then \( f_{G_1} = 2 \). Suppose that \( f_{21}, f_{22}, f_{23}, \) and \( f_{24} \) are hexagons, pairwise different, and intersecting if and only if \( f_{22} \) and \( f_{2i+1} \) are intersecting at only one edge for \( i = 1, 2, 3, 4 \), \( f_{25} = f_{21} \). Set \( G_2 = G_1 \cup \{f_{21}, f_{22}, f_{23}, f_{24}\} \). Suppose \( f_{21}, f_{22}, f_{23}, \) and \( f_{24} \) are the inner faces of \( G_2 \), and let \( f_{31}, f_{32}, f_{33}, f_{34}, f_{35}, \) and \( f_{36} \) be six neighboring faces of \( G_2 \) along the clockwise direction, such that \( f_{31} \) is incident with the two consecutive 2-degree vertices on \( \partial(G_2) \) (see Figure 2c). Then \( f_{G_2} = 2 + 4 = 6 \).

![Figure 2](image-url)

Suppose that the proposition holds for any integer less than \( n \), where \( n > 2 \). According to the induction hypothesis, \( f_{G_{n-1}} = n^2 - n \) and \( f_{n1}, f_{n2}, \ldots, f_{n2n} \) are \( 2n \) neighboring faces of \( G_{n-1} \) along the clockwise direction, such that \( f_{ni} \) is incident with the two consecutive 2-degree vertices on \( \partial(G_{n-1}) \). Suppose that \( f_{ni1}, \ldots, f_{ni2n} \) are hexagons, pairwise different, and intersecting if and only if \( f_{ni} \) and \( f_{ni+1} \) are intersecting at only one edge for \( i = 1, 2, \ldots, 2n \), \( f_{n2n+1} = f_{n1} \). Set \( G_n = G_{n-1} \cup \{f_{ni1}, \ldots, f_{ni2n}\} \). Suppose \( f_{ni1}, \ldots, f_{ni2n} \) are all inner faces of \( G_n \) (see Figure 3). Then \( f_{G_n} = n^2 - n + 2n = n^2 + n, n \in \mathbb{Z} \).
Proposition 2. In all the (2,6)-fullerenes, there exists a fragment, say $C_n$, such that $f_{C_n} = n$, $n \in \mathbb{Z}$.

Proof. Let $C_0$ be $3 \times K_2$, then $f_{C_0} = 0$. Let $d_1$ and $d_2$ be two 2-length faces. Its boundary, $\partial(d_i)$, is labelled $v_1^i, v_2^i$ ($i = 1, 2$). Let $P_i$ be a path that connects two vertices, $v_1^i$ and $v_2^i$ ($i = 1, 2$), and $V(P_1) \cap V(P_2) = \emptyset$. If both $P_1$ and $P_2$ are 2-paths, then, as $F$ is 2-connected, there is a fragment, $f_1$, such that $f_1$ contains the paths $P_1$ and $P_2$ and the edges $v_1^i v_2^j$ and $v_2^i v_3^j$. Set $C_1 = d_1 \cup d_2 \cup f_1$, without loss of generality, suppose $f_1$ is the inner face of $C_1$ (see Figure 4a). Thus, $f_{C_1} = 1$. If both $P_1$ and $P_2$ are 4-paths, then all whose internal vertices are denoted by $x_1, x_2, x_3, y_1, y_2, y_3$, respectively, such that $P_1 = v_1^1 x_1 x_2 x_3 v_1^2$ and $P_2 = v_2^1 y_1 y_2 y_3 v_2^2$. Let $x_2 y_2 \in E(F)$, then there are 2 hexagons, denoted by $f_1$ and $f_2$, such that $\partial(f_1) = v_1^1 v_2^1 y_1 x_2 x_1 v_1^2$ and $\partial(f_2) = v_2^1 x_1 x_2 y_1 y_2 v_2^2$. Set $C_2 = d_1 \cup d_2 \cup f_1 \cup f_2$, also suppose $f_1$ and $f_2$ are two inner faces of $C_2$ (see Figure 4b), then $f_{C_2} = 2$. Suppose $P_1$ and $P_2$ are 2n-paths, $n \in \mathbb{N}^+$. Let $P_1 = v_1^1 x_1 \ldots x_{2n-1} v_1^2$ and $P_2 = v_2^1 y_1 \ldots y_{2n-1} v_2^2$. Suppose that $x_i y_i \in E(F)$ ($i = 2, 4, \ldots, 2n - 2$), then there are $n$ hexagons between $P_1$ and $P_2$, denoted by $f_1, f_2, \ldots, f_n$. Set $C_n = d_1 \cup d_2 \cup \bigcup_{i=1}^{n} f_i$, such that $f_1, f_2, \ldots, f_n$ are the inner faces of $C_n$ (see Figure 4c). Therefore, $C_n$ is a fragment and $f_{C_n} = n$, $n \in \mathbb{N}^+$. Thus, there exists a fragment, $C_n$, such that $f_{C_n} = n$, $n \in \mathbb{Z}$.

Figure 4. The fragments $C_1$ (a), $C_2$ (b), and $C_n$ (c).

Proposition 3. In all the (2,6)-fullerenes, there exists a fragment, say $L_n^m$, such that $f_{L_n^m} = 2n^2 + (m + 3)n$, $n \in \mathbb{N}^+, m \in \mathbb{Z}$.

Proof. Let $G_n'$ and $G_n''$ be two fragments, as indicated in Figure 3. By Proposition 1, we know that $G_n'$ and $G_n''$ both have $n^2 + n$ hexagons. Suppose $n$ is a positive integer. Since there are $2n + 2$ 2-degree vertices on $\partial(G_n')$, we can record them clockwise as $u_1, u_2, \ldots, u_{2n + 2}$, such that $u_1$ and $u_{2n + 2}$ are adjacent. Similarly, $2n + 2$ 2-degree vertices on $\partial(G_n'')$ are denoted by $v_1, v_2, \ldots, v_{2n+2}$ along the ant clockwise direction of $G_n''$, such that $v_1$ and $v_{2n+2}$ are adjacent. For $G_n'$ and $G_n''$. Let $e_1 = u_1 v_1, e_2 = u_2 v_2$, then $e_1$ and $e_2$ are contained in the hexagon, say $f_1$. Set $K_1 = G_n' \cup G_n'' \cup f_1$ (see Figure 5a), then $f_{K_1} = 5$. For $C_n'$ and $C_n''$. Let $e_i = u_i v_i, i = 1, 2 \ldots n + 1$, then $e_i$ and $e_{i-1}$ are contained in the hexagon, say $f_i, i = 1, 2 \ldots n$.
Set $K_n = G' \cup G'' \bigcup_{i=1}^{n} f_i$, suppose all of $f_1 \ldots f_n$ are the inner faces of $K_n$ (see Figure 5b, the embedding of $K_n$), then $f_{K_n} = 2(n^2 + n) + n = 2n^2 + 3n$.

Next, we construct the fragment $L_n^m$ from $K_n$ as follows. We replace each edge, $e_i = u_iv_i$, by a path, $P_i$, such that $P_i = u_i x_1 x_2 \ldots x_m v_i$, $i = 1, 2, \ldots n + 1$, $m \in \mathbb{Z}$. Suppose that $x_2 x_{i+1,1}, x_4 x_{i+1,3} \ldots x_{2m} x_{i+1,2m-1}$ be the edges of $F$, $i = 1, 2 \ldots n$. Therefore, there are $m + 1$ hexagons between $P_i$ and $P_{i+1}$, denoted by $f_1, f_2 \ldots f_{i+1}$, $i = 1, 2 \ldots n$. Set $L_n^m = G' \cup G'' \bigcup_{i=1}^{m} \{f_1, f_2 \ldots f_{i+1}\}$, $m \in \mathbb{Z}$ (see Figure 5c, the embedding of $L_n^m$). Therefore, $L_n^m$ is a fragment and $f_{L_n^m} = 2(n^2 + n) + (m + 1)n = 2n^2 + (m + 3)n$, $n \in \mathbb{N}^+, m \in \mathbb{Z}$. \(\square\)

![Figure 5](image-url)

**Figure 5.** The fragments $K_1$ (a), $K_n$ (b), and $L_n^m$ (c).

**Proposition 4.** In all the $(2, 6)$-fullerenes, there exists a fragment, say $H_n$, such that $f_{H_n} = 2n + 2$, $n \in \mathbb{Z}$.

**Proof.** Let $H_0 \cong F_6$ be the $(2, 6)$-fullerene with six vertices. Without loss of generality, suppose the exterior face of $H_0$ is a 2-length face with the boundary $u_1v_1u_1$, and the remaining two 2-length faces are connected by an edge, $u_2v_2$ (see Figure 6a, the embedding of $H_0$ and the labelling of $u_1, v_1, u_2, v_2$). Next, we construct the fragment $H_n$ from $H_0$ as follows: we replace the two parallel edges, $u_1v_1$, and one edge, $u_2v_2$, by two paths, $P_1$ and $P_3$, and one path, $P_5$, such that $P_i = u_i x_1 x_2 \ldots x_{2n} v_i$, $i = 1, 2, 3$. Set $x_2 x_{i+1,1}, x_4 x_{i+1,3} \ldots x_{2n} x_{i+1,2n-1}$ be the edges of $F$, $i = 1, 2$. We construct $n + 1$ hexagons between $P_i$ and $P_{i+1}$, denoted by $f_1, f_2 \ldots f_{i+1}$, $i = 1, 2$. Set $H_n = H_0 - \{u_1v_1, u_2v_2\} \bigcup_{i=1}^{n} \{f_1, f_2 \ldots f_{i+1}\}$, such that $f_1, f_2 \ldots f_{i+1}$ are the inner faces of $H_n$, $n \in \mathbb{N}^+$ (see Figure 6b). Therefore, $H_n$ is a fragment and $f_{H_n} = 2(n + 1) = 2n + 2$, $n \in \mathbb{N}^+$. Thus, there exists a fragment, $H_n$, such that $f_{H_n} = 2n + 2, n \in \mathbb{Z}$. \(\square\)

![Figure 6](image-url)

**Figure 6.** The fragments $H_0$ (a) and $H_n$ (b).

By Propositions 1–4, we can find a $(2, 6)$-fullerene $F$ having $f_F$ hexagonal faces that relates to the parameters $n$ and $m$.

**Theorem 7.** There exists a $(2, 6)$-fullerene $F$ such that $f_F = n^2 + 2n$, $n \in \mathbb{Z}$.

**Proof.** Let $G_n$ be a fragment of $F$, as shown in Figure 3. Its boundary, $\partial(G_n)$, is labelled $u_1, u_2, \ldots, u_{4n+2}$ along the clockwise direction, where $u_1$ and $u_2$ are two consecutive 2-degree vertices. Let $C_n$ be a fragment of $F$, as shown in Figure 4c. Its boundary, $\partial(C_n)$,
is labelled \(v_1, v_2, \ldots, v_{4n+2}\) along the clockwise direction, where \(v_1\) and \(v_2\) are two consecutive 3-degree vertices. Next, we assume each of the graphs \(G_n\) and \(C_n\) drawn on a hemisphere, with the boundary as equator. If \(\partial(G_n) = \partial(C_n)\), then set \(F = G_n \cup C_n\). By Propositions 1 and 2, then \(f_F = f_{G_n} + f_{C_n} = n^2 + 2n, n \in \mathbb{Z}\). \(\square\)

**Theorem 8.** There exists a \((2,6)\)-fullerene \(F\) such that \(f_F = 3n^2 + m^2 + 3mn + 6n + 3m + 2, n \in \mathbb{N}^+, m \in \mathbb{Z}\).

**Proof.** Let \(G_{m+n+1}\) be a fragment of \(F\), as shown in Figure 3. Its boundary, \(\partial(G_{m+n+1})\), is labelled \(u_1, u_2, \ldots, u_{4m+4n+6}\) along the clockwise direction, where \(u_1\) and \(u_2\) are two consecutive 2-degree vertices. Let \(L_n^m\) be a fragment of \(F\), as shown in Figure 5C. Its boundary, \(\partial(L_n^m)\), is labelled \(v_1, v_2, \ldots, v_{4m+4n+6}\) along the clockwise direction, where \(v_1\) and \(v_2\) are two consecutive 3-degree vertices. Next, we assume each of the graphs \(G_{m+n+1}\) and \(L_n^m\) drawn on a hemisphere, with the boundary as equator. If \(\partial(G_{m+n+1}) = \partial(L_n^m)\), then set \(F = G_{m+n+1} \cup L_n^m\). By Propositions 1 and 3, then \(f_F = f_{G_{m+n+1}} + f_{L_n^m} = 3n^2 + m^2 + 3mn + 6n + 3m + 2, n \in \mathbb{N}^+, m \in \mathbb{Z}\). \(\square\)

**Theorem 9.** There exists a \((2,6)\)-fullerene \(F\) such that \(f_F = n^2 + 3n + 2, n \in \mathbb{Z}\).

**Proof.** Let \(G_n\) be a fragment of \(F\), as shown in Figure 3. Its boundary, \(\partial(G_n)\), is labelled \(u_1, u_2, \ldots, u_{4n+2}\) along the clockwise direction, where \(u_1\) and \(u_2\) are two consecutive 2-degree vertices. Let \(H_n\) be a fragment of \(F\), as shown in Figure 6b. Its boundary, \(\partial(H_n)\), is labelled \(v_1, v_2, \ldots, v_{4n+2}\) along the clockwise direction, where \(v_1\) and \(v_2\) are two consecutive 3-degree vertices. Next, we assume each of the graphs \(G_n\) and \(H_n\) drawn on a hemisphere, with the boundary as equator. If \(\partial(G_n) = \partial(H_n)\), then set \(F = G_n \cup H_n\). By Propositions 1 and 4, then \(f_F = f_{G_n} + f_{H_n} = n^2 + 3n + 2, n \in \mathbb{Z}\). \(\square\)

### 3. Conclusions

In this paper, we characterized the structural properties of \((2,6)\)-fullerenes \(F\). By the conclusion of Došlić on \((k,6)\)-fullerenes, we know that every \((2,6)\)-fullerene is 1-extendable, and then, by means of the relationship between the extendable and resonance, we know that every \((2,6)\)-fullerene is 1-resonant. But, by the definition of \(n\)-extendable, we find that every \((2,6)\)-fullerene is not 2-extendable, and then not \(k\)-extendable \((k \geq 3)\). Moreover, we find that no \((2,6)\)-fullerene is bicritical. On the other hand, for the anti-Kekulé number of \((2,6)\)-fullerene \(F\), we firstly obtain the upper bound 4 of the anti-Kekulé number of \(F\) by the definition of an anti-Kekulé set. Secondly, with the help of Tutte’s Theorem, and combing with the structure of \((2,6)\)-fullerene, we obtain the lower bound 3 of the anti-Kekulé number of \(F\). Finally, by analyzing that the anti-Kekulé number of \(F\) cannot be 3, we find that the anti-Kekulé number of \(F\) is 4.

Grünaub and Motzkin showed that \((5,6)\)-fullerene and \((4,6)\)-fullerene having \(n\) hexagonal faces exist for every non-negative integer, \(n\), satisfying \(n \neq 1\), and showed a similar result for \((3,6)\)-fullerene. Therefore, at the end of the paper, we consider whether \((2,6)\)-fullerene having \(n\) hexagonal faces also exists for any \(n\). We try to give a positive answer to this question, but we find that the conclusion seems quite elusive. So, we mainly prove that there exists a \((2,6)\)-fullerene \(F\) having \(f_F\) hexagonal faces, where \(f_F\) is related to the two parameters \(n\) and \(m\). There are, however, still several important open questions.

**Problem 1.** Whether every \((2,6)\)-fullerene is \(k\)-resonant \((k \geq 2)\)?

**Problem 2.** Whether for every \(n \neq 1\) there exists a \((2,6)\)-fullerene \(F\) such that \(f_F = n\)?

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