

Article

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_F hexagonal faces, where f_F is related to the two parameters n and m .

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



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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 graph 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 $C = xyx$. 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 $|V(F)| > 2$. $\square$

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

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

By (1), we obtain that

$$l' = 4f'_2 - 2. \quad (2)$$

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]. Combining 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 $v_1v_2v_1$. 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.

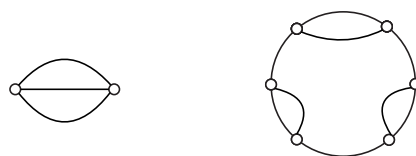
For the connected cubic simple bipartite graph, we know its anti-Kekulé number is 4 [22].

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 .



(a) $3 \times K_2$

(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 , and 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 , and 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, $\bigcup_{i=1}^{|S|+2} F_i$ sends out exactly $\sum_{i=1}^{|S|+2} d(F_i) - 2ak(F)$ edges to N . Hence

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

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

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

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 W and B are the bipartition of F . By Hall's theorem, there exists $U \subseteq W$ such that

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

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 ,

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

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

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

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. $\square$

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_{2i} and $f_{2,i+1}$ 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 $f_{G_2} = 2 + 4 = 6$.

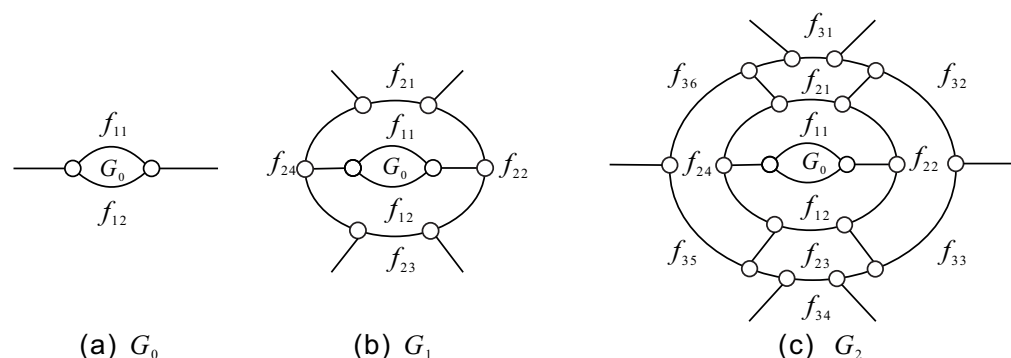


Figure 2. The fragments G_0 (a), G_1 (b), and G_2 (c).

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 $f_{n1}, f_{n2}, \dots, f_{n,2n}$ are $2n$ neighboring faces of G_{n-1} along the clockwise direction, such that f_{n1} is incident with the two consecutive 2-degree vertices on $\partial(G_{n-1})$. Suppose that $f_{n1}, \dots, f_{n,2n}$ are hexagons, pairwise different, and intersecting if and only if f_{ni} and $f_{n,i+1}$ are intersecting at only one edge for $i = 1, 2, \dots, 2n$, $f_{n,2n+1} = f_{n1}$. Set $G_n = G_{n-1} \cup \{f_{n1}, \dots, f_{n,2n}\}$. Suppose $f_{n1}, \dots, f_{n,2n}$ are all inner faces of G_n (see Figure 3). Then $f_{G_n} = n^2 - n + 2n = n^2 + n$, $n \in \mathbb{Z}$. $\square$

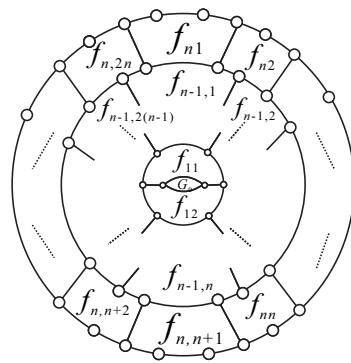


Figure 3. The fragment G_n .

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_{i1}, v_{i2} ($i = 1, 2$). Let P_i be a path that connects two vertices, v_{i1} and v_{i2} ($i = 1, 2$), 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 hexagon, say f_1 , such that f_1 contains the paths P_1 and P_2 and the edges $v_{11}v_{12}$ and $v_{21}v_{22}$. 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 and y_1, y_2, y_3 , respectively, such that $P_1 = v_{11}x_1x_2x_3v_{21}$ and $P_2 = v_{12}y_1y_2y_3v_{22}$. Let $x_2y_2 \in E(F)$, then there are 2 hexagons, denoted by f_1 and f_2 , such that $\partial(f_1) = v_{11}v_{12}y_1y_2x_2x_1v_{11}$ and $\partial(f_2) = v_{21}x_3x_2y_2y_3v_{22}v_{21}$. 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 $P_1 = v_{11}x_1 \dots x_{2n-1}v_{21}$ and $P_2 = v_{12}y_1 \dots y_{2n-1}v_{22}$. Suppose that $x_iy_i \in E(F)$ ($i = 2, 4, \dots, 2n-2$), then there are n hexagons between P_1 and P_2 , denoted by $f_1, f_2 \dots f_n$. Set $C_n = d_1 \cup d_2 \cup \bigcup_{i=1}^n f_i$, such that $f_1, f_2 \dots f_n$ 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 $f_{C_n} = n$, $n \in \mathbb{Z}$. $\square$

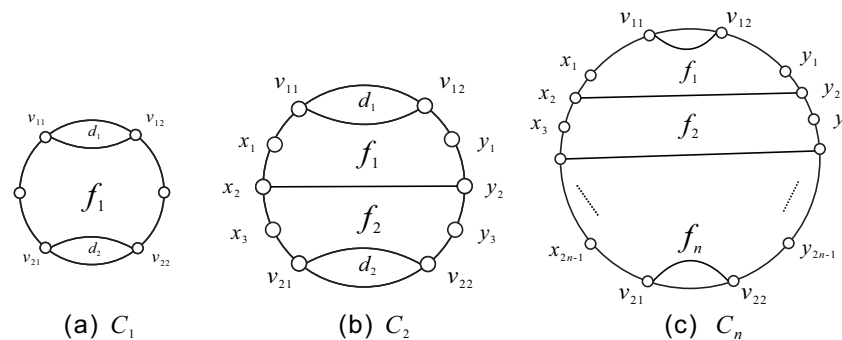


Figure 4. The fragments C_1 (a), C_2 (b), and C_n (c).

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 $u_1, u_2, \dots, u_{2n+2}$, such that u_1 and u_{2n+2} are adjacent. Similarly, $2n + 2$ 2-degree vertices on $\partial(G''_n)$ are denoted by $v_1, v_2, \dots, v_{2n+2}$ along the anticlockwise direction of G''_n , such that v_1 and v_{2n+2} are adjacent. For G'_1 and G''_1 . Let $e_1 = u_1v_1, e_2 = u_2v_2$, then e_1 and e_2 are contained in the hexagon, say f_1 . Set $K_1 = G'_1 \cup G''_1 \cup f_1$ (see Figure 5a), then $f_{K_1} = 5$. For G'_n and G''_n . Let $e_i = u_iv_i, i = 1, 2 \dots n + 1$, then e_i and e_{i+1} are contained in the hexagon, say $f_i, i = 1, 2 \dots n$.

Set $K_n = G'_n \cup G''_n \cup_{i=1}^n f_i$, suppose all of $f_1 \dots f_n$ 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, $e_i = u_i v_i$, by a path, P_i , such that $P_i = u_i x_{i1} x_{i2} \dots x_{i,2m} v_i$, $i = 1, 2 \dots n+1$, $m \in \mathbb{Z}$. Suppose that $x_{i2} x_{i+1,1}, x_{i4} x_{i+1,3} \dots x_{i,2m} x_{i+1,2m-1}$ be the edges of F , $i = 1, 2 \dots n$. Therefore, there are $m+1$ hexagons between P_i and P_{i+1} , denoted by $f_{i1}, f_{i2} \dots f_{i,m+1}$, $i = 1, 2 \dots n$. Set $L_n^m = G'_n \cup G''_n \cup_{i=1}^n \{f_{i1}, f_{i2} \dots f_{i,m+1}\}$, $m \in \mathbb{Z}$ (see Figure 5c, the embedding of L_n^m). Therefore, L_n^m is a fragment and $f_{L_n^m} = 2(n^2 + n) + (m+1)n = 2n^2 + (m+3)n$, $n \in \mathbb{N}^+$, $m \in \mathbb{Z}$. $\square$

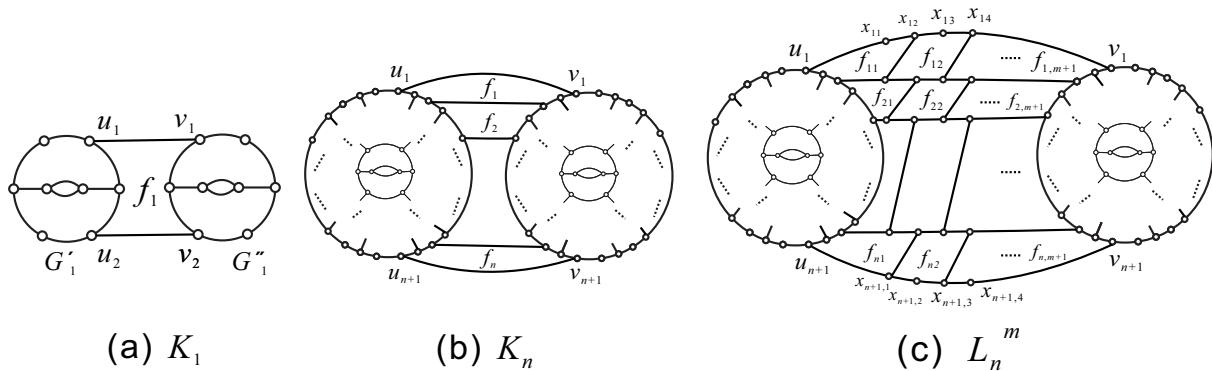


Figure 5. The fragments K_1 (a), K_n (b), and L_n^m (c).

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 $u_1 v_1 u_1$, and the remaining two 2-length faces are connected by an edge, $u_2 v_2$ (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, $u_1 v_1$, and one edge, $u_2 v_2$, by two paths, P_1 and P_3 , and one path, P_2 , such that $P_i = u_i x_{i1} x_{i2} \dots x_{i,2n} v_i$, $i = 1, 2$, and $P_3 = u_1 x_{31} x_{32} \dots x_{3,2n} v_1$, $n \in \mathbb{N}^+$. Suppose that $x_{i2} x_{i+1,1}, x_{i4} x_{i+1,3} \dots x_{i,2n} x_{i+1,2n-1}$ be the edges of F , $i = 1, 2$. We construct $n+1$ hexagons between P_i and P_{i+1} , denoted by $f_{i1}, f_{i2} \dots f_{i,n+1}$, $i = 1, 2$. Set $H_n = H_0 - \{u_1 v_1, u_2 v_2\} \cup_{i=1}^2 \{f_{i1}, f_{i2} \dots f_{i,n+1}\}$, such that $f_{i1}, f_{i2} \dots f_{i,n+1}$ 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 $f_{H_n} = 2n + 2$, $n \in \mathbb{Z}$. $\square$

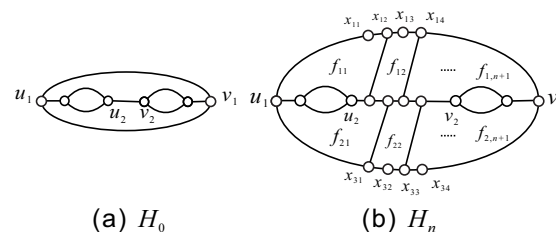


Figure 6. The fragments H_0 (a) and H_n (b).

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 $u_1, u_2, \dots, u_{4n+2}$ 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 $v_1, v_2, \dots, v_{4n+2}$ 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 $u_1, u_2, \dots, u_{4m+4n+6}$ 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 $v_1, v_2, \dots, v_{4m+4n+6}$ 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 $u_1, u_2, \dots, u_{4n+2}$ 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 $v_1, v_2, \dots, v_{4n+2}$ 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 $(2,6)$ -fullerene 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 combining 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.

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 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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