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On Resonance of (4,5,6)-Fullerene Graphs*

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Abstract

A (4,5,6)-fullerene graph is a plane cubic graph all of whose faces are only quadrilaterals, pentagons and hexagons. For a (4,5,6)-fullerene graph F, an even face (or cycle) is called resonant if its boundary (or itself) is an M-alternating cycle for some perfect matching M of F. In this paper, we prove that every (4,5,6)-fullerene graph with at least one pentagon is cyclically 4-edge connected, and thus bicritical. We mainly show that each quadrilateral face of a (4,5,6)-fullerene graph is resonant and all hexagonal faces are resonant except for three classes of (4,5,6)-fullerene graphs which are characterized as nanotubes with three quadrilaterals and six pentagons. Further, we show that all the resonant 6-cycles in (4,5,6)-fullerenes are just formed from all hexagonal faces except for one hexagon in the mentioned-above three types of nanotubes, and from all pairs of quadrilaterals with a common edge.

1 Introduction

Since the first fullerene, Buckminsterfullerene C_{60}, was discovered by Kroto et al. [16] in 1985, fullerenes have aroused great interest and extensive attention among researchers and lead to the formation of fullerene science. It is generally accepted that fullerenes or classical fullerenes in chemical literature are plane (or spherical) cubic graphs in structures whose faces are pentagons and hexagons [20], which are thus called (5,6)-fullerenes. By Euler's polyhedron formula, every fullerene with n atoms has exactly 12 pentagons and $(n/2-10)$ hexagons.

However, several theoretical studies demonstrated that non-classical fullerenes with four-membered rings cannot be dismissed in advance. Gao and Herndon [13] investigated

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non-classical fullerenes with quadrilaterals by the SCF-UHF calculations and molecular mechanics and found that some non-classical fullerene isomers with fewer than 60 carbon atoms may actually be stabilized by incorporation of two four-membered rings. Babić and Trinajstić [3] systematically generated all fullerenes with four-membered rings on from 20 to 60 carbon atoms by modifying the well-known spiral code method. One can see that the presence of four-membered rings greatly enriches the world of fullerenes. They used the topological resonance energy (TRE) method [1, 14] and the conjugated circuits model (CC) [19] to select the most stable isomers, which contain at least one four-membered ring except for Buckministerfullerene C_{60}. The results are only qualitative as none of the models accounts for strain. Further, Fowler et al. [10] and Zhao et al. [32] respectively computed energies of all fullerene isomers with four-membered rings of C_{40} and C_{32} and obtained similar conclusions.

In addition, boron-nitrogen fullerenes and nanotubes have emerged in experimental evidence, see [4, 7, 9, 21]. The former has (4,6)-fullerene graph as molecular graph with exactly six quadrilateral faces and other hexagonal faces.

The structural properties and isomer stabilities of (5,6)-fullerenes and (4,6)-fullerenes were extensively investigated from both chemical and mathematical points of view. For mathematical aspects of fullerenes, one can refer to a recent survey [2] and references within it. In particular, (5,6)-fullerenes have the cyclical edge-connectivity 5 and (4,6)-fullerenes have the cyclical edge-connectivity 4 or 3 [8, 18]. Both (5,6)-fullerenes and (4,6)-fullerenes with the cyclical edge-connectivity 4 are 2-extendable graphs [28, 30]. For benzenoid systems and fullerenes, conjugated or resonant hexagons (alternate in single and double bonds within a Kekulé structure) play an important role in Clar's aromatic sextet theory [6] and Randić's conjugated circuit model [19]. It is known that all hexagons and quadrilaterals in (4,6)- and (5,6)-fullerenes are resonant [25, 28]. For other works on resonant faces of various plane graphs, see refs. [5, 12, 15, 23, 24, 26, 27, 29, 31, 33].

To our knowledge, a systematic study on non-classical fullerenes with four-, five- and six-membered rings has not been found in mathematics. Precisely, we can define a (4,5,6)-fullerene (graph) to be a plane (or spherical) cubic graph whose faces are only quadrilaterals, pentagons and hexagons, which obviously includes all (4,6)- and (5,6)-fullerenes.

In this paper we start such a study on general (4,5,6)-fullerene graphs. In the next section we recall some concepts and results needed in our discussions. In Section 3, we will prove that each (4,5,6)-fullerene graph is 3-connected. This confirms that the (4,5,6)-fullerene graphs can be polyhedral graphs. Further, every (4,5,6)-fullerene graph with at least one pentagon is cyclically 4-edge connected, and thus bicritical (the removal of any pair of distinct vertices results in a subgraph with a perfect matching). The latter shows a chemical consequence that every derivative of a (4,5,6)-fullerene graph with a pentagon by substituting any two carbon atoms permits still a Kekulé structure. In Section 4 we show that every quadrilateral face of a (4,5,6)-fullerene graph is resonant and find actually some examples of (4,5,6)-fullerenes with a non-resonant hexagonal face. Our main result is to determine all the three types of (4,5,6)-fullerenes with a non-resonant hexagonal face h as zigzag nanotubes by adding the same cap consisting of one hexagon h and the six pentagons along it on one end and three distinct caps with three quadrilaterals on the other end. For details, see Theorem 4.3 and Fig. 3. Finally, we present structures of all 6-cycles in (4,5,6)-fullerene graphs as the boundaries of four patches (see Lemma 5.1). Further, we show that all the resonant 6-cycles of (4,5,6)-fullerenes are just formed from all hexagonal faces except for the hexagon h in the mentioned-above three types of nanotubes, and from all pairs of quadrilaterals with a common edge.

2 Preliminaries

Throughout this paper, we only consider finite, simple and connected plane graph $G = (V(G), E(G), F(G))$, where $V(G)$ denotes the vertex set, $E(G)$ the edge set and $F(G)$ the face set of G. We follow the definition and terminology in [17] unless otherwise stated.

For a (4,5,6)-fullerene G with n vertices, let p_i denote the number of faces (including exterior faces) with i-sides of G, $i = 4, 5, 6$. Fowler et al. [10] got the following equalities,

$$|F(G)| = n/2 + 2, \tag{1}$$

$$2p_4 + p_5 = 12, \tag{2}$$

$$p_6 = (n - p_5)/2 - 4. \tag{3}$$

What's more, G has $|F(G)| = p_4 + p_5 + p_6 \geq p_4 + p_5 = 6 + \frac{p_5}{2} \geq 6$ faces. Thus, $n = 2(|F(G)| - 2) \geq 8$ by Eq. (1). As we know, a (4,6)-fullerene exists for all even number $n \geq 8$ except $n = 10$ [9], while a (5,6)-fullerene exists for every even number $n \geq 20$ except $n = 22$ [11]. For the other special case $p_6 = 0$, a (4,5)-fullerene graph has

$n = 8 + p_5 \leq 20$ vertices by Eq. (3). We can show that there are only six (4,5)-fullerene graphs, see Fig. 1. Hence, a (4,5,6)-fullerene graph with n vertices exists for every even number $n \geq 8$, and the cube is the smallest (4,5,6)-fullerene graph.

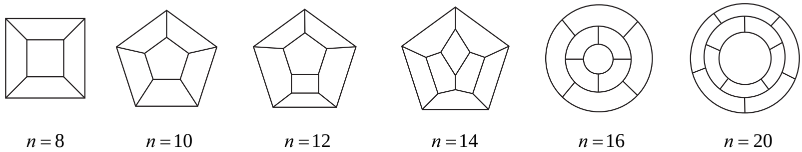


Figure 1. The six (4,5)-fullerene graphs.

The degree of any vertex $v \in V(G)$, denoted by $d_G(v)$ (or $d(v)$ for short), is the number of all neighbors of v. If $d_G(v) = 1$, then we call v a *pendent vertex* of G and the edge incident with v a *pendent edge*. For a subset $E_0 \subseteq E(G)$, $G - E_0$ is the subgraph of G by deleting the edges of E_0. H is called a *subgraph* of G, written by $H \subseteq G$, when $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. For $H \subseteq G$, $G - H$ is the subgraph of G obtained by deleting the vertices of $V(H)$ together with the edges incident with vertices in H.

An edge set M of a graph G is called a *matching* if any two edges of M have no an endvertex in common. A *perfect matching* (or Kekulé structure in chemical literature) of G is a matching such that every vertex is incident with one edge of it. A bipartite graph G is said to be *elementary* if it is connected and each edge lies in a perfect matching of G. A connected graph G with at least $2k + 2$ vertices is said to be *k-extendable* if it has a matching with size k and each such matching can be always contained in some perfect matching of G. If $G - x - y$ has a perfect matching for any two distinct vertices x and y of G, then G is *bicritical*. An even cycle of G is called *resonant* if there exists a perfect matching M such that it is an *M-alternating* cycle (i.e., the edges of the cycle alternate in M and $E(G) \setminus M$). For a plane graph G, a face is called *resonant* if its boundary is a resonant cycle, and a cycle is a *facial cycle* if it is the boundary of a face.

Let $S \subseteq V(G)$ and $\overline{S} = V(G) \setminus S$. Denoted by $[S, \overline{S}]$ the set of edges of G with one endvertex in S and the other one in $\overline{S}$. If both S and $\overline{S}$ are nonempty, then we call $[S, \overline{S}]$ a *k-edge cut* of G if $|[S, \overline{S}]| = k$. The *edge connectivity* of a graph G, denoted by $\kappa'(G)$, is equal to the minimum cardinality of edge cuts. An edge cut of G is called *trivial* if all edges of it are incident with a common vertex. A l-cycle means a cycle with length l.

An edge cut E_1 of a connected graph G is called a *cyclical edge cut* if at least two components of $G - E_1$ contain cycles. The *cyclical edge-connectivity* of G, denoted by $c\lambda(G)$, is the minimum number of any cyclical edge cut. Graph G is called cyclically k-edge connected if $c\lambda(G) \geq k$.

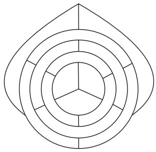


Figure 2. Illustration for a (4,6)-fullerene graph T_3.

A $(k,6)$-cage ($k \geq 3$ is an integer) is a 3-connected cubic planar graph whose faces are only k-gons and hexagons. Let T_n denote the (4,6)-fullerene graph that consists of n concentric layers of hexagons and capped on each end by a cap T^0 formed by three quadrangles with one common vertex. For example, see T_3 in Fig. 2. Let $\mathcal{T} = \{T_n | n \geq 1\}$. Došlić gave the following result.

Theorem 2.1 ([8]). *Let G be a $(k,6)$-cage. Then G only exists for $k = 3, 4$ and 5. Moreover, $c\lambda(G) = 3$ if $G \in \mathcal{T}$, otherwise, $c\lambda(G) = k$.*

3 Preliminary results

For a (4,6)-fullerene graph, it was proved that it has the connectivity 3 [28]. Hence a (4,6)-fullerene graph is always a (4,6)-cage. By an analogous manner, we have the following general result.

Lemma 3.1. *Every (4,5,6)-fullerene graph F has the connectivity 3.*

Proof. Since every cubic graph has an equal vertex and edge connectivity, it suffices to prove that $\kappa'(F) = 3$. Since every edge of F belongs to a quadrilateral, pentagon or hexagon, there is no cut edge in F. That is, $\kappa'(F) \geq 2$. This implies that F has no 3-cycles since every 3-cycle of F must be a facial cycle, a contradiction.

Suppose $\kappa'(F) = 2$. Then F has a 2-edge cut. So we choose one $E_0 = \{e_1, e_2\}$ such that $|V(F_1)|$ is as small as possible, where F_1 and F_2 are the two components of $F - E_0$. Obviously, F_1 does not contain any 2-edge cut of F. Let C_i be the boundary of the face of F_i but not a face of F and $||C_i||$ the length of the walk along C_i, $i = 1, 2$. Let u_j and v_j be the endvertices of e_j lying on C_1 and C_2, respectively, for $j = 1, 2$. Then, F_1 (resp. F_2) has exactly two vertices u_1 and u_2 (resp. v_1 and v_2) with degree 2 and the other vertices with degree 3. So both F_1 and F_2 have a cycle. We have that u_1 is not adjacent to u_2; otherwise, the two edges of F_1 incident with u_1 and u_2 other than u_1u_2 will be a 2-edge cut of F, a contradiction. If u_1 and u_2 have the same two neighbors in F_1, then either the two neighbors are adjacent and a triangle face happens or two edges incident with the two neighbors form a 2-edge cut of F, which would be both impossible. So, $||C_1|| \geq 5$. On the other hand, the total size of two faces of F whose boundaries contain both e_1 and e_2 can be expressed as $||C_1|| + ||C_2|| + 4 \leq 12$ as there is no face of F with more than 6 sides, which implies that $||C_2|| \leq 3$ and a triangle happens, a contradiction.

Therefore, $\kappa'(F) \geq 3$, and the desired result $\kappa'(F) \leq 3$ holds since the three edges incident with any vertex of F form an edge cut of F. ■

Lemma 3.2. *Let F be a (4,5,6)-fullerene graph. Then F has no 3-cycles and every 4- or 5-cycle of F is a facial cycle.*

Proof. From Lemma 3.1 and its proof we know that $\kappa'(F) = 3$ and F has no 3-cycles respectively. Let C be a l-cycle of F, where $l = 4$ or 5. We claim that C is a facial cycle. Otherwise, both E_1 and E_2 are not empty, where E_1 and E_2 denote the sets of edges pointing towards the interior and exterior of C, respectively. Further no edge of E_1 and E_2 connects two vertices of C, otherwise a triangle happens, a contradiction. Hence both E_1 and E_2 are edge cuts of F and $|E_1| + |E_2| = l \leq 5$, which implies that one of E_1 and E_2 contains at most two edges, contradicting $\kappa'(F) = 3$. ■

Next, we will study that the cyclical edge-connectivity of (4,5,6)-fullerene graphs with at least one quadrilateral and one pentagon (for the other cases, see Theorem 2.1), which is critical for proving our main results.

Theorem 3.3. *Let F be a (4,5,6)-fullerene graph with at least one quadrilateral and one pentagon. Then $c\lambda(F) = 4$.*

Proof. By Lemma 3.1, F is 3-edge connected, and thus $c\lambda(F) \geq 3$. On the other hand, $c\lambda(F) \leq 4$ as F contains faces with 4 sides and F has at least 6 faces. It suffices to show that $c\lambda(F) \neq 3$.

Suppose, to the contrary, that F has a cyclical 3-edge cut E_0. Let F_1 and F_2 be the two components of $F - E_0$. We may suppose that the outer face of F is just the outer face of F_2. Then F_1 lies in an inner face f of F_2. Let C_1 the boundary of the outer face of F_1 and C_2 the boundary of f. From the 3-connectivity of F we know that E_0 is a matching of F which is between C_1 and C_2, C_i $(i = 1, 2)$ are cycles, and both F_1 and F_2 are 2-connected.

It is obvious that each C_i $(i = 1, 2)$ has exactly three vertices incident with the edges in E_0. Let k_1 and k_2 be the number of additional vertices on C_1 and C_2, respectively. Since F has no face with more than 6 sides, the three faces of F bounded by two edges in E_0 each has at most two additional vertices on C_1 and C_2. Hence $k_1 + k_2 \leq 6$.

Claim 1. $k_1 = k_2 = 3$.

To get the claim it suffices to prove that $k_1 \geq 3$ and $k_2 \geq 3$. Suppose to the contrary that $k_1 \leq 2$. Since F has no triangles by Lemma 3.2, $k_1 \geq 1$. If $k_1 = 1$, then there is a cut edge of F in the interior of C_1, a contradiction. If there are two additional vertices on C_1, then there must be no edge connecting them, otherwise there would be a triangle, a contradiction. Hence, there are two edges from the two additional vertices towards the interior of C_1, which form a 2-edge cut, contradicting the 3-connectedness of F. Similarly, we have that $k_2 \geq 3$. So the claim is confirmed.

From Claim 1 and the restriction on faces of F we immediately obtain that the three faces of F between C_1 and C_2 are hexagons. Let E_0' denote the set of edges from the 3 additional vertices on C_1 pointing towards the interior of C_1. Since F is 3-connected, E_0' is a 3-edge cut of F. If E_0' is a trivial 3-edge cut of F, then F_1 is a cap formed by three quadrilaterals with one common vertex, and the three additional vertices on C_1 (also on C_2) are pairwise nonadjacent by Lemma 3.2.

Now we may choose the above E_0 as a cyclical 3-edge cut of F such that $|V(F_1)|$ is as small as possible in the sequel. From the above discussions we know that E_0' is a 3-edge cut of F. We assert that E_0' is a trivial 3-edge cut. Otherwise, let F_1' denote one component of $F - E_0'$ contained in the interior of C_1. By the above choice we know that F_1' is a tree. If $|V(F_1')| \geq 2$, then there are at least four edges between F_1' and C_1 since there are at least two pendent vertices in F_1', a contradiction. So the assertion holds and F_1 is formed by three quadrilaterals with one common vertex.

We now consider F_2. Let E_1 be the set of edges of F_2 incident with the three additional vertices on C_2 and towards the exterior of C_2. If E_1 is not a cyclical edge cut, then, similar as the analysis of E_0', we can get that E_1 is a trivial edge cut, i.e., there is only one vertex in the exterior of C_2. Thus, F_2 is formed by three quadrilaterals with one common vertex. Hence, $F = T_1 \in \mathcal{T}$. But if E_1 is a cyclical 3-edge cut, then similar as the analysis of C_1 or C_2, we can get that the boundary C_3 of the face of F_3 but not a face of F is a cycle, where F_3 is one component of $F - E_1$ contained in the exterior of C_2. By Claim 1, we can get that the three faces of F between C_2 and C_3 are hexagons and there is also another 3-edge cut E_2 of F incident with the three additional vertices on C_3 and towards the exterior of C_3. If E_2 is not a cyclical edge cut, then, similar as the analysis of E_0', we can get that E_2 is also a trivial edge cut, i.e., there is only one vertex in the exterior of C_3. Thus, F_3 is formed by three quadrilaterals with one common vertex. Hence, $F = T_2 \in \mathcal{T}$. But if E_2 is a cyclical 3-edge cut, then similar as the analysis of C_1 or C_2, we can also get that the boundary C_4 of the face of F_4 but not a face of F is also a cycle, where F_4 is one component of $F - E_2$ contained in the exterior of C_3. Then, by Claim 1, we can also get that the three faces of F between C_3 and C_4 are hexagons and there is also another 3-edge cut E_3 of F incident with the three additional vertices on C_4 and towards the exterior of C_4. Thus, by the finiteness of F, we can do this operation repeatedly until the mth step such that E_m is a 3-edge cut but not a cyclical edge cut of F. Then, similar as the analysis of E_0', we can get that there is exactly one vertex in the exterior of the cycle C_{m+1}, i.e., $F = T_m \in \mathcal{T}$. In conclusion, if $c\lambda(F) = 3$, then $F \in \mathcal{T}$, a contradiction to the hypothesis. ■

Combining Theorems 2.1 and 3.3, we can easily get the following result.

Corollary 3.4. *A (4,5,6)-fullerene graph is cyclically 4-edge connected if and only if it does not belong to* $\mathcal{T}$.

Corollary 3.5. *Every 3-edge cut of a (4,5,6)-fullerene graph but not in* $\mathcal{T}$ *is trivial.*

Proof. Let F be such a (4,5,6)-fullerene graph and E_0 be any 3-edge cut of F. By Lemma 3.1, F is 3-connected. Assume that G_1 and G_2 are the two components of $F - E_0$. Since F is 3-regular, $|V(G_i)|$ is odd, where $i = 1, 2$. Suppose, to the contrary, that $|V(G_i)| \geq 3$ for $i = 1, 2$. Then, $|E(G_i)| = \frac{3|V(G_i)|-3}{2} = |V(G_i)| + \frac{|V(G_i)|-3}{2} \geq |V(G_i)|$, i.e., there is a cycle in G_i, $i = 1, 2$. Hence, $c\lambda(F) = 3$, a contradiction by Corollary 3.4. ■

Lemma 3.6 ([28]). *Every (4,6)-fullerene graph is 1-extendable.*

Lemma 3.7 ([17]). *For some integer $k \geq 3$, if G is k-regular, cyclically $(k+1)$-edge-connected and has an even number of points, then G is bicritical or elementary bipartite.*

Corollary 3.8. *Every (4,5,6)-fullerene graph is 1-extendable. Further, every (4,5,6)-fullerene graph with at least one pentagon is bicritical.*

Proof. It is immediate from Corollary 3.4 and Lemmas 3.6 and 3.7. ■

4 Main results

Let F_n^i be the (4,5,6)-fullerene graph consisting of caps P_0 and P_i $(1 \leq i \leq 3)$, and n concentric layers of hexagons between them; see Fig. 3. We mention that the cap P_0 is formed by a hexagon, say h, and six pentagonal faces around it. Let $\mathscr{F}_i = \{F_n^i | n \geq 0\}$, $1 \leq i \leq 3$. Clearly, each $F \in \mathscr{F}_i$ has exactly six pentagonal and three quadrilateral faces which lie in caps P_0 and P_i, $1 \leq i \leq 3$.

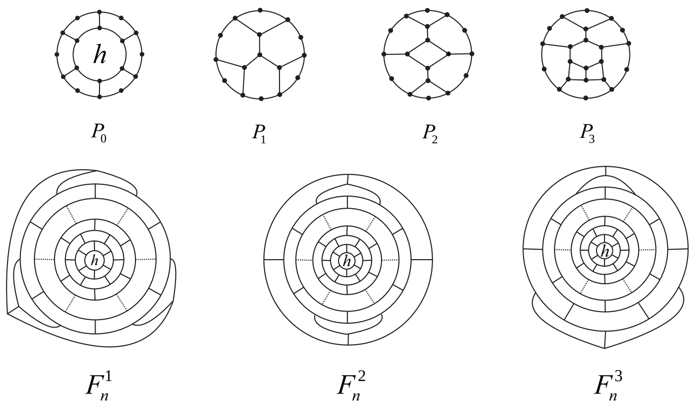


Figure 3. Illustration for graphs F_n^1, F_n^2 and F_n^3.

To get our main result, we first state Tutte's Theorem [17] as follows.

Theorem 4.1. *A graph G has a perfect matching if and only if $c_0(G-S) \leq |S|$ for any set $S \subseteq V(G)$, where $c_0(G-S)$ is the number of odd components of $G-S$.*

Lemma 4.2 ([28]). *Every face of $F \in \mathcal{T}$ is resonant.*

Theorem 4.3. *Let F be a (4,5,6)-fullerene graph. Then*

(i) *each quadrilateral face in F is resonant, and*

(ii) *each hexagonal face in F is resonant if and only if $F \notin \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$.*

Proof. By Lemma 4.2, we only need to consider the case $F \notin \mathcal{T}$, that is, F is cyclically 4-edge connected by Corollary 3.4.

By Lemma 3.1, we have that F is 3-connected. Let $C = u_1u_2 \cdots u_l u_1$ be the facial cycle of an even face f in F and $F_0 = F - V(C)$. Then, $|V(F_0)|$ is even. Suppose that f is not resonant. By Theorem 4.1, there exists a set $X_0 \subseteq V(F_0)$ such that $\alpha = c_0(F_0 - X_0) \geq |X_0| + 1$. Since α and $|X_0|$ have the same parity, $\alpha \geq |X_0| + 2$. Let $G_1, \ldots, G_{\alpha+\beta}$ be the components of $F_0 - X_0$, where G_i $(1 \leq i \leq \alpha)$ are odd components and G_j $(\alpha+1 \leq j \leq \alpha+\beta)$ are even components. Let m_i be the number of edges between G_i and X_0, γ_i be the number of edges between G_i and C and γ_0 be the number of edges between X_0 and C, $1 \leq i \leq \alpha+\beta$. Then $\sum_{i=0}^{\alpha+\beta} \gamma_i = l$ and $m_i + \gamma_i \geq 3$ as F is 3-connected, $1 \leq i \leq \alpha + \beta$.

Therefore,

$$\begin{aligned} 3(\alpha+\beta) &\leq \sum_{i=1}^{\alpha+\beta}(m_i+\gamma_i) = \Big(\sum_{i=1}^{\alpha+\beta} m_i + \gamma_0\Big) + \sum_{i=0}^{\alpha+\beta}\gamma_i - 2\gamma_0 \\ &\leq 3|X_0| + \sum_{i=0}^{\alpha+\beta}\gamma_i - 2\gamma_0 \\ &\leq 3(\alpha-2) + l - 2\gamma_0 = 3\alpha + l - 6 - 2\gamma_0. \end{aligned} \tag{4}$$

(i) If f is a quadrilateral, then we have $l = 4$. Hence, by Ineq. (4), we have

$$3(\alpha+\beta) \;\; \leq \;\; 3\alpha - 2 - 2\gamma_0,$$

i.e., $3\beta \leq -2 - 2\gamma_0$, a contradiction. Hence, every quadrilateral face of F is resonant.

(ii) Suppose that f is a hexagon. Then $l = 6$. Thus, by Ineq. (4), we have

$$3(\alpha+\beta) \;\; \leq \;\; 3\alpha - 2\gamma_0,$$

which implies that $\beta = 0, \gamma_0 = 0$ and all equalities in Ineq. (4) always hold. The first equality in Ineq. (4) holds if and only if $m_i + \gamma_i = 3$, $1 \leq i \leq \alpha$. Then, by Corollary 3.5, we have $|V_{G_i}| = 1$, $1 \leq i \leq \alpha$. Without loss of generality, let Y_0 denote the set of all singletons G_i, $1 \leq i \leq \alpha$. The second equality in Ineq. (4) holds if and only if there is no any edge in the subgraph $F_0[X_0]$, which implies that X_0 is an independent set of F_0. Hence, $F_0 = (X_0, Y_0)$ is bipartite. And the third equality in Ineq. (4) holds if and only if $\alpha = |X_0| + 2$. For the sake of clarity, we color the vertices of X_0 and Y_0 by white and black, respectively.

By Corollary 3.5 and the 3-connectedness of F, we can easily get that F_0 is connected. By Lemma 3.2 and Corollary 3.5, the set of edges between C and F_0 is a matching of F, i.e., no two edges of this set share an endvertex. So, F_0 has exactly six vertices with degree 2 and the remaining vertices with degree 3. Since $\gamma_0 = 0$, we have that all vertices of F_0 with degree 2 belong to Y_0. Without loss of generality, we can assume that v_i is the vertex of F_0 with degree 2 and adjacent to u_i in F, $1 \leq i \leq 6$.

Since the distance between v_i and v_{i+1} in F_0 is even, the face along the path $v_i u_i u_{i+1} v_{i+1}$ is a pentagonal face as every face of F is at most 6 sides, i.e., there is exactly one vertex $x_i \in X_0$ adjacent to v_i and v_{i+1}, where the subscripts are taken mod 6, $i = 1, 2, \ldots, 6$. By Lemma 3.2, any two vertices x_j and x_k with $j \neq k$ are different and there is no edge connecting them as F_0 is bipartite, $1 \leq j, k \leq 6$. Let $V' = \{x_1, \ldots, x_6\}$ and $V'' = \{v_1, \ldots, v_6\}$. Then, $H = F[V(C) \cup V' \cup V'']$ is a cap formed by a hexagon f and six pentagons around f. What's more, the outer face of H is of size 12 with six 2-degree vertices and six 3-degree vertices alternating on its facial cycle, see Fig. 4.

Let $\bar{H} = F - H$. Then there is no isolated vertex in $\bar{H}$. Otherwise, assume v is an isolated vertex of $\bar{H}$. Then, by the 3-connectedness of F, the neighbors of v in H must be three successive vertices of V', say x_1, x_2 and x_3. Thus, the face along the path $x_6 v_1 x_1 v x_3 v_4 x_4$ is at least 8 sides as the distance between x_6 and x_4 in $\bar{H}$ is even, a contradiction. If there is no pendent vertex in $\bar{H}$, then, similarly as the above analysis

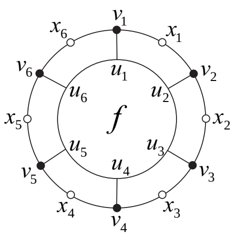


Figure 4. Illustration for induced subgraph H in Theorem 4.3.

of H at the beginning of (ii), we can get that the layer, say L_1, along H consists of six hexagons.

Let $H_1 = F[V(H) \cup V(L_1)]$. Then, the outer face of H_1 is also of size 12 with six

2-degree vertices and six 3-degree vertices alternating on its facial cycle. Let $\bar{H}_1 = F - H_1$. Then, similar to $\bar{H}$, there is also no isolated vertex in $\bar{H}_1$. If there is also no pendent vertex in $\bar{H}_1$, then, similar as the analysis of H, we can also get that the layer L_2 along H_1 consists of six hexagons. Let $H_2 = F[V(H) \cap V(L_1) \cap V(L_2)]$. Then, the outer face of H_2 is also of size 12 with six 2-degree vertices and six 3-degree vertices alternating on its facial cycle. Thus, we can do this operation repeatedly until the $(m+1)$th step such that the subgraph $\bar{H}_m = F - H_m$ has pendent vertices, where $H_m = F[V(H) \cup V(L_1) \cup \cdots \cup V(L_m)]$. We may suppose that $C_m = v'_1 x'_1 \cdots v'_6 x'_6 v'_1$ is the facial cycle of the outer face of H_m and $x'_i \in X_0$ and $v'_i \in Y_0$ are those vertices with degree 2 and 3 in H_m, respectively, $1 \le i \le 6$. Similar as the analysis of $\bar{H}$, we can also get that $\bar{H}_m$ has no isolated vertex and at most three pendent vertices. Note that if v is a pendent vertex of $\bar{H}_m$, then by the 3-connectedness and planarity of F, v must be adjacent to two successive vertices of $\{x'_1, \ldots, x'_6\}$. Next, we proceed by considering the following possible cases.

Case 1. There are exactly three pendent vertices in $\bar{H}_m$. Then the three pendent edges of $\bar{H}_m$ form a 3-edge cut of F. By Corollary 3.5, we have $\bar{H}_m \cong K_{1,3}$. Thus, we can get the other cap P_1 of F, i.e., $F = F^1_m \in \mathscr{F}_1$.

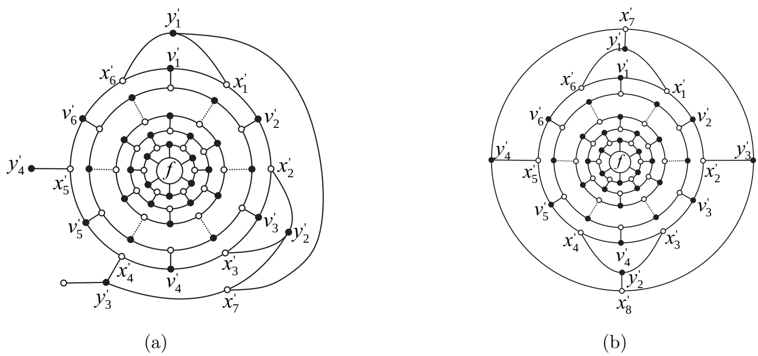


Figure 5. Illustration for the proof of Case 2 of Theorem 4.3.

Case 2. There are only two pendent vertices in $\bar{H}_m$, say y'_1 and y'_2. Without loss of generality, we can suppose that y'_1 is adjacent to x'_1 and x'_6. We claim that y'_2 is adjacent to x'_3 and x'_4.

Suppose, to the contrary, that y'_2 is adjacent to x'_2 and x'_3. Assume that y'_3 and y'_4 are the vertices of $\bar{H}_m$ that are adjacent to x'_4 and x'_5, respectively, as depicted in Fig. 5(a).

Since the face along the path $y_2'x_3'v_4'x_4'y_3'$ is at most 6 sides and the distance between y_2' and y_3' in $\bar{H}_m$ is even, there is a path $y_2'x_7'y_3'$, where $x_7' \in X_0$. Moreover, y_1' is also adjacent to x_7' by considering the face along $y_1'x_1'v_2'x_2'y_2'x_7'$. But, in this case, the size of the face along the path $y_4'x_5'v_6'x_6'y_1'x_7'y_3'$ is at least 8, a contradiction. Similarly, y_2' is not adjacent to x_4' and x_5'. Thus, our claim is verified.

Hence, y_2' is adjacent to x_3' and x_4'. In this case, we may assume that y_3' and y_4' in $\bar{H}_m$ are adjacent to x_2' and x_5', while x_7' and x_8' are adjacent to y_1' and y_2' in $\bar{H}_m$, respectively, as depicted in Fig. 5(b). Obviously, $x_7' \neq x_8'$ by Lemma 3.1. Since the face along the path $x_7'y_1'x_1'v_2'x_2'y_3'$ is at most 6 sides and the distance between x_7' and y_3' in $\bar{H}_m$ is odd, x_7' is adjacent to y_3'. Similarly, y_3' is also adjacent to x_8' and y_4' is adjacent to both x_7' and x_8'. Thus, we get the other cap P_2 of F, i.e., $F = F_m^2 \in \mathscr{F}_2$.

Case 3. There is exactly one pendent vertex in $\bar{H}_m$, say y_1'. Without loss of generality, suppose that y_1' is adjacent to x_1' and x_6', see Fig. 6.

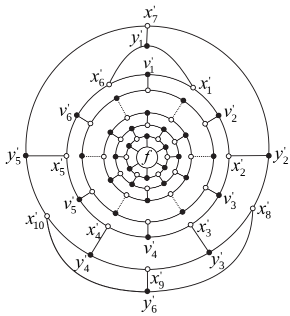


Figure 6. Illustration for the proof of Case 3 in Theorem 4.3.

Suppose that $y_i' \in V(\bar{H}_m)$ is a neighbor of x_i', $2 \leq i \leq 5$. Since the face along the path $y_1'x_1'v_2'x_2'y_2'$ is at most 6 sides and the distance between y_1' and y_2' in $\bar{H}_m$ is even, there is a path $y_1'x_7'y_2'$, where $x_7' \in X_0$. By the same reasoning, x_7' is also adjacent to y_5'. Furthermore, y_i' and y_{i+1}' also have a common neighbor, say x_{6+i}', $2 \leq i \leq 4$. By the 3-connectedness of F, any two vertices of $\{x_8', x_9', x_{10}'\}$ are different and there is also no edge connecting any two of them as $\bar{H}_m \subseteq F_0$ is bipartite. Then, the three edges incident with x_8', x_9' and x_{10}' form a trivial edge cut of F by Corollary 3.5. Thus, we get the other cap P_3, that is, $F = F_m^3 \in \mathscr{F}_3$.

In conclusion, if a hexagonal face f of F is not resonant, then $F \in \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$.

Conversely, suppose $F \in \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$. We will show that the hexagonal face h of F, as depicted in Fig. 3, is not resonant, that is, $F - h$ has no perfect matchings. Let (X_0, Y_0) be the bipartition of bipartite graph $F - h$. Since $F - h$ has exactly six 2-degree vertices which belong to the same class, say X_0, while the remaining vertices with degree 3, we have that $|E(F - h)| = 3(|X_0| - 6) + 12 = 3|Y_0|$. That is, $|X_0| = |Y_0| + 2$, which implies that $F - h$ has no perfect matchings by Theorem 4.1.

Therefore, statement (ii) of the theorem holds. ■

From the above proof, we can see that each graph in $\mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$ has a unique non-resonant hexagonal face h in the cap P_0.

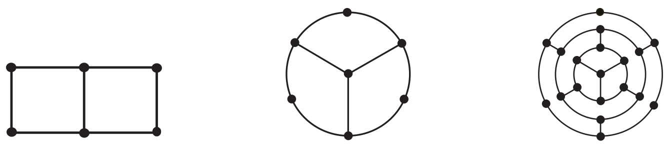
Since there are exactly six pentagons and three quadrilaterals in any (4,5,6)-fullerene graph $F \in \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$, we get the following result immediately by Theorem 4.3.

Corollary 4.4. *[25] Every hexagonal face of (5,6)-fullerene graphs is resonant.*

5 Concluding remarks

From Lemma 3.2, we have that every 4-cycle is a facial cycle of a (4,5,6)-fullerene graph, but not all 6-cycles are facial cycles. Now we give the possible structures of all 6-cycles in a (4,5,6)-fullerene graph. In fact, all cases of 6-cycles of (4,6)-fullerene graphs have been characterized [22]. However, all 6-cycles of (5,6)-fullerenes are boundaries of faces [25].

We call the three structures in Fig. 7 dual-square, square-cap and a square-cap with 2 hexagon-layers, respectively. In fact, we have a square-cap with k ($k \geq 1$) hexagon-layers.



(a) dual-square (b) square-cap (c) a square-cap with 2 hexagon-layers

Figure 7. Illustration for three types of 6-cycle in (4,5,6)-fullerene graphs.

Lemma 5.1. *Let F be a (4,5,6)-fullerene graph with a 6-cycle C. Then C is the boundary of either a hexagonal face, or a dual-square, or a square-cap, or a square-cap with hexagon-layers. Further, the later two cases appear only in a tube $F \in \mathcal{T}$ or the cube.*

Proof. Suppose that C is not a hexagonal facial cycle. If C has a chord (i.e., an edge e whose endvertices both lie on C, but e dos not in C), then, by Lemmas 3.1 and 3.2, C is the boundary of a dual-square. Otherwise, let E_1 and E_2 be the sets of edges pointing towards the interior and exterior of C from C, respectively. By Lemma 3.1, both E_1 and E_2 are 3-edge cuts of F.

If F is cyclically 4-edge connected, then both E_1 and E_2 are trivial 3-edge cuts by Corollary 3.5. Thus, C is the boundary of a square-cap and F is a cube. Otherwise, $c\lambda(F) = 3$, at least one of E_1 and E_2 is a cyclical edge cut, and $F \in \mathcal{T}$ by Theorem 2.1 and Corollary 3.4. Further, by the proof of Theorem 3.3 we can see that C is the boundary of a square-cap or a square-cap with hexagon-layers. ■

By Theorem 4.3, we know that not all hexagonal faces of (4,5,6)-fullerene graphs are resonant. Next, we will give all resonant 6-cycles of (4,5,6)-fullerene graphs.

Theorem 5.2. *Let F be a (4,5,6)-fullerene graph. Then a 6-cycle of F is resonant if and only if it is either a facial cycle except for h in $F \in \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$, or the boundary of a dual-square.*

Proof. Let C be a 6-cycle. By Lemma 5.1, C is the boundary of either a hexagonal face, or a dual-square, or a square-cap, or a square-cap with hexagon-layers.

For the case of dual-square, we can show that C is resonant in an almost the same method as the proof (i) of Theorem 4.3. Here there are also four edges leaving from C.

For the boundary C of a hexagonal face, C is always resonant precisely except for h in $F \in \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3$ by Theorem 4.3.

For the other cases, we may suppose that C is the boundary of a square-cap with n hexagon-layers, where $n \geq 0$. Obviously, $F - V(C)$ has an odd component with $(6n + 1)$ vertices. This implies that $F - V(C)$ has no perfect matchings, that is, C is not resonant. ■

Combining Lemma 5.1 with Theorem 5.2, we can get the following result.

Corollary 5.3. *Let F be a (4,5,6)-fullerene graph. Then F contains a non-resonant 6-cycle if and only if F is a cube or $F \in \mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3 \cup \mathcal{T}$.*

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