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Hexagonal resonance of (3,6)-fullerenes

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Abstract A (3,6)-fullerene G is a plane cubic graph whose faces are only triangles and hexagons. It follows from Euler's formula that the number of triangles is four. A face of G is called *resonant* if its boundary is an alternating cycle with respect to some perfect matching of G. In this paper, we show that every hexagon of a (3,6)-fullerene G with connectivity 3 is resonant except for one graph, and there exist a pair of disjoint hexagons in G that are not mutually resonant except for two trivial graphs without disjoint hexagons. For any (3,6)-fullerene with connectivity 2, we show that it is composed of $n(n \geq 1)$ concentric layers of hexagons, capped on each end by a cap formed by two adjacent triangles, and none of its hexagons is resonant.

Keywords (3,6)-fullerene · Perfect matching · Resonant hexagon

1 Introduction

For $k \geq 3$ an integer, a $(k, 6)$-*fullerene* is a planar cubic graph whose faces are only k-gons and hexagons. The only values of k for which $(k, 6)$-fullerene exists are 3, 4 and 5. A (4,6)-fullerene is a boron-nitrogen fullerene molecular graph and a (5,6)-fullerene is the ordinary carbon fullerene molecular graph. Inspired by the boron-nitrogen and carbon fullerenes, we naturally want to investigate (3,6)-fullerene graph G.

A (3,6)-fullerene graph G has the same connectivity and edge-connectivity 2 or 3. The structure of a (3,6)-fullerene G with connectivity 3 is well know [7–9], namely,

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it is determined by only 3 parameters r, s, t, where r is the radius (number of rings), s is the size (number of spokes = twice the number of steps), and t is the twist (torsion, $-s < t \leq s, t \equiv r \bmod 2$). For the (3,6)-fullerenes with connectivity 2, the structure has not been characterized yet. In Sect. 2 of this paper we prove that the (3,6)-fullerenes with connectivity 2 consist of $n(n \geq 1)$ concentric layers of hexagons, capped on each end by a cap formed by two adjacent triangles.

In [8], P.R. Goodey also indicated that any (3,6)-fullerene with connectivity 3 admitted a hamiltonian circuit. Moreover, it is known that every (3,6)-fullerene is 1-extendable [16], and we can see that none of the (3,6)-fullerenes is 2-extendable similar to Lemma 4.4 of [13] since every (3,6)-fullerene is a cubic graph with a triangle. A *matching* of a graph G is a set of disjoint edges M of G, and a *perfect matching* is a matching M covering all vertices of G. A connected graph G is n-*extendable*$(|V(G)| \geq 2n+2)$ if any matching of n edges is contained in a perfecting matching of G.

In physical and chemical context, physicist and chemist are interested in the energy spectra of (3,6)-fullerenes which determine their electronic and magnetic properties [1,22]. The *spectrum* of a graph is the collection of eigenvalues of its adjacency matrix together with their multiplicity. In 1995, P.W. Fowler [7] conjectured that the spectrum of any (3,6)-fullerene with connectivity 3 has the form: $\{3, -1, -1, -1; \lambda_1, \lambda_2, \ldots, \lambda_{\frac{n}{2}-2}; -\lambda_1, -\lambda_2, \ldots, -\lambda_{\frac{n}{2}-2}\}$, where n is the number of vertices of the graph. In 2009, DeVos et al. [4] confirmed the conjecture for all (3,6)-fullerenes by Cayley sum graphs. Meantime, applying the results of toroidal fullerenes to (3,6)-fullerenes, John and Sachs [12] explicitly calculated the eigenvalues for the (3,6)-fullerenes with connectivity 3, and proved the conjecture.

This paper is mainly concerned with the hexagonal resonance of (3,6)-fullerenes, i.e. the property that any given hexagon is an aromatic sextet. This concept of "resonance" originates from Clar's aromatic sextet theory [3] and Randić's conjugated circuit model; see also [17,18]. A face of a plane graph G is called *resonant* if its boundary is an alternating cycle with respect to some perfect matching M of G (i.e., the edges of its boundary appear alternately in and off M). In [25], Zhang and Chen showed that each hexagon of a normal (1-extendable) hexagonal system is resonant. Later, Zhang and Zheng [26] gave a similar characterization for generalized hexagonal systems (i.e., the hexagonal systems with some "holes"; see also [2,10]). Zhang and Zhang [30] generalized this result to plane elementary bipartite graph: each face of a plane bipartite graph G is resonant if and only if G is 1-extendable. This result is suitable for open-ended carbon nanotubes [27], boron-nitrogen fullerenes [28], cubic bipartite polyhedral graphs [21] and polygonal systems [15]. For plane non-bipartite graphs, Ye et al. [24] proved that every hexagon of a fullerene graph is resonant. A natural question arises: does this result still hold for the (3,6)-fullerenes? The present paper gives a complete answer in Sects. 2 and 3 which is somewhat different from that of the fullerenes: 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.

A set $\mathcal{H}$ of disjoint hexagons of G is called a *resonant pattern* (or *sextet pattern)* if G has a perfect matching M such that each hexagon in $\mathcal{H}$ is M-alternating. A (3,6)-fullerene G is k-*resonant* (or k-*coverable*, $k \geq 1$) if any $i (0 \leq i \leq k)$ disjoint hexagons of G form a resonant pattern. In Sect. 3 we also show that the only two 2-resonant

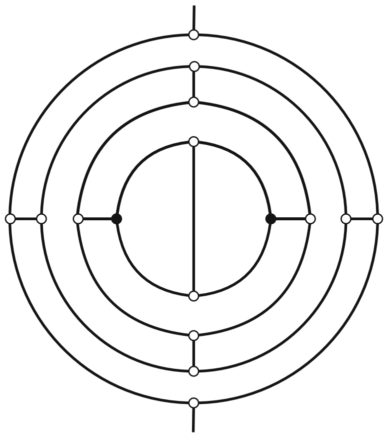


Fig. 1 A (3,6)-fullerene T_3

(3,6)-fullerenes are trivial, that is, both of them have no two disjoint hexagons, thus are also k-resonant for all integer $k \geq 2$. For more details on resonance theory, please see [11,14,19,20,29,31,32].

Given a plane embedding of G, we say that two faces of G are *adjacent* if they share an edge. Triangular and hexagonal faces are referred to simply as triangles and hexagons. Let C be a cycle in G. We denote by $I[C]$ the subgraph of G consisting of the cycle C together with its interior. We say two vertices of G are *on the same side of* C if they are simultaneously in the interior or the exterior of C. Moreover, in a cubic plane graph, each vertex is incident with exactly three faces and two adjacent faces share at least one edge.

2 (3,6)-fullerenes with connectivity 2

Let $T_n (n \geq 1)$ be the graph consisting of n concentric layers of hexagons, capped on each end by a cap formed by two adjacent triangles (see Fig. 1). We can see $T_n (n \geq 1)$ are the (3,6)-fullerenes with connectivity 2.

Before starting our main results, we give a simple structural lemma to the cycle of a (3,6)-fullerene.

Lemma 2.1 *Let G be a (3,6)-fullerene and C a cycle in G with the boundary $v_1, v_2, \ldots, v_n$ along the clockwise direction of C. Let v_i' be the neighbor of v_i other than v_{i-1} and v_{i+1}, where the subscripts are taken mod n, $i = 1, 2, \ldots, n$.*

(i) *If $n \geq 4$ and v_2' and v_3' are on the same side of C, then the four vertices v_1, v_2, v_3, v_4 must be contained in the same hexagon (see* Fig. 2a*) and C has length at least five.*

(ii) *If $n = 4$ and v_1', v_3' are on the same side of C, and v_2', v_4' are on the other side of C, then $G \cong T_n$ for some $n \geq 1$ or $G \cong K_4$ (the complete graph with four vertices).*

(iii) *If $n = 3$, then v_1', v_2' and v_3' must be on the same side of C.*

Proof (i) Since v_1, v_2, v_3 and v_4 lie on the boundary of a face of G, they must be contained in the same hexagon. If C is a cycle with length 4, then

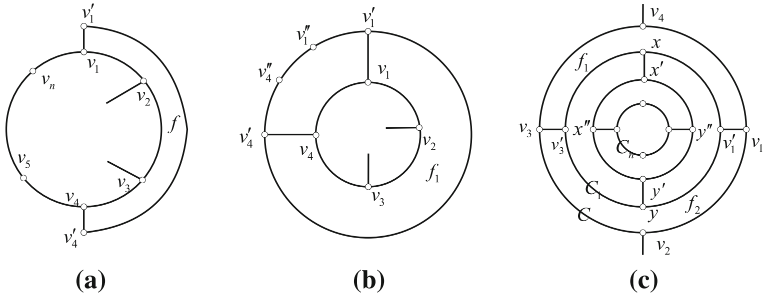


Fig. 2 **a** the four vertices v_1, v_2, v_3, v_4 contained in the same hexagon, **b** a forbidden subgraph for (3,6)-fullerenes, and **c** an illustration to the case (ii)

$C = v_1v_2v_3v_4v_1$ and $v_1'v_1v_2v_3v_4v_4'v_1'$ is the boundary of a hexagonal face f_1 (see Fig. 2b). Without loss of generality, suppose v_2' and v_3' are in the interior of C. Then v_1' and v_4' must be in the exterior of C. Otherwise, there will be a cut set of size one or a face of size four in G, contradicting the definition of (3,6)-fullerene. Then we obtain a cycle $v_1'v_1v_4v_4'v_1'$ denoted by C_1, which satisfies the conditions of (i) (see Fig. 2b). Applying the same method to the 4-length cycle C_1, we obtain a series of 4-length cycles $C_1, C_2, \ldots, C_n, \ldots$, each satisfying the conditions of (i), and the process cannot stop, which is impossible.

(ii) Without loss of generality, suppose v_1', v_3' are in the interior of C. To obtain the structure of G, by the symmetry it suffices to discuss the structure of $I[C]$. If v_1 is adjacent to v_3, then we obtain a cap formed by two adjacent triangles. Otherwise, $v_1'v_1v_4v_3v_3'xv_1'$ and $v_1'v_1v_2v_3v_3'yv_1'$ are the boundaries of two hexagonal faces by Lemma 2.1 (i), where x and y are the common neighbors of v_1' and v_3' (see Fig. 2c). Now we can use the same method to the cycle C_1 with the boundary $v_1'yv_3'xv_1'$. Because of the finiteness of G, after a finite number of steps, say n, we will obtain a cycle C_n of length 4 which will have no vertices of G in its interior. Then the two vertices of degree two on the boundary of C_n must be adjacent and we obtain a cap formed by two adjacent triangles. Applying the same method to the cycle C and its exterior we will obtain that $G \cong T_n$ for some $n \geq 1$ or $G \cong K_4$ (the case when v_1 is adjacent to v_3 and v_2 is adjacent to v_4).

(iii) Suppose v_1', v_2' and v_3' are not on the same side of C. Then we obtain a cut set of size one in G, contradicting the face that G is 2-connected. □

Theorem 2.2 *The connectivity of a (3,6)-fullerene G is 2 if and only if $G \cong T_n$ for some $n \geq 1$.*

Proof We can see that T_n, $n \geq 1$, has a vertex cut of two vertices. So it has connectivity 2. It suffices to prove the "only if" part.

Let G be a (3,6)-fullerene with connectivity 2 and a 2-vertex cut $S = \{u, v\}$. Suppose that H_1 and H_2 are two components of $G - S$. For the sake of clarity, we color the vertices of H_1 and H_2 by white and black, respectively. By the 3-regularity and planarity of G, we have the following claims:

Claim 1 u and v each has at least one neighbor in each component of $G - S$. Furthermore, u (and v) together with its two neighbors both of which belong to different components are contained in the same hexagonal face f whose boundary contains the vertex v (and u).

Proof Suppose to the contrary that there exists one component not containing any neighbors of u (or v). Then the vertex v (or u) forms a vertex cut, contradicting the 2-connectedness of G.

The second claim can be easily obtained by the planarity of G and the fact that there are no edges between $V(H_1)$ and $V(H_2)$. □

Claim 2 There are exactly two components of $G - S$.

Proof At most three components of $G - S$ can be obtained by Claim 1 and the 3-regularity of G. If there exist three components H_1, H_2, H_3 of $G - S$, then by Claim 1 each neighbor of u (and v) belongs to exactly one of $V(H_1)$, $V(H_2)$ and $V(H_3)$, that is, precisely two edges are sent out from S to H_j and H_j is 2-edge-connected by the 2-connectedness of G for $j = 1, 2, 3$. Let $j \in \{1, 2, 3\}$. There are precisely two vertices of degree two on the boundary of H_j while the remaining vertices of $V(H_j)$ with degree three are in the interior of H_j. Let $|V(H_j)| = n_j$ and $|E(H_j)| = m_j$. Denote by $f_j(3)$ and $f_j(6)$ the number of triangular and hexagonal faces in H_j, respectively. Then the total number of faces in H_j is $f_j(3) + f_j(6) + 1$. On the other hand, $2m_j = 3n_j - 2 = 3f_j(3) + 6f_j(6) + l$, where l is the length of the exterior face of H_j. Then we obtain that $m_j = 3n_j/2 - 1$ and $f_j(6) = (3n_j - 2 - l - 3f_j(3))/6$. Substituting these values into the Euler formula, $n_j - m_j + f_j(3) + f_j(6) + 1 = 2$, we have $f_j(3) = (l + 2)/3$. Since G is 2-connected, the only values of $l \geq 2$ that yield integer $f_j(3)$ are 4, 7 and 10, and the corresponding values of $f_j(3)$ are 2, 3 and 4, respectively. That is, H_j has at least two triangles and the total number of triangles in G is not less than six, contradicting the fact that G has exactly four triangles. So there exist precisely two components of $G - S$, as claimed. □

Denote by b_1, w_1, x_1 the three neighbors of u. By Claims 1 and 2, we assume that w_1 and b_1 belong to $V(H_1)$ and $V(H_2)$, respectively. Let $abcb_1uw_1a$ be the boundary of f along the clockwise direction. Then $v = a$, or b, or c.

Claim 3 u is not adjacent to v.

Proof To the contrary, suppose u and v are adjacent. Whatever $v = a$, or b, or c, all are conflict with Lemma 2.1 (see Fig. 3a, b and c). This contradiction completes the proof of Claim 3. □

As noted earlier, we fulfill the proof of Theorem 2.2 in three cases in u and v nonadjacent conditions: $v = c$, or b, or a.

If $v = c$, then u is not adjacent to b or a. Otherwise, there will be a 4-length cycle or a 3-length cycle, both of which contradict Lemma 2.1 (see Fig. 4a and b). Similarly, v is not adjacent to a or w_1, and w_1 is not adjacent to b. By Claim 2, x_1 belongs to either $V(H_1)$ or $V(H_2)$. If x_1 belongs to $V(H_1)$, then x_1, u and b_1 must be contained in the same hexagon (say f_1) whose boundary contains the vertex v by Claim 1 and $x_1 \neq a, b$

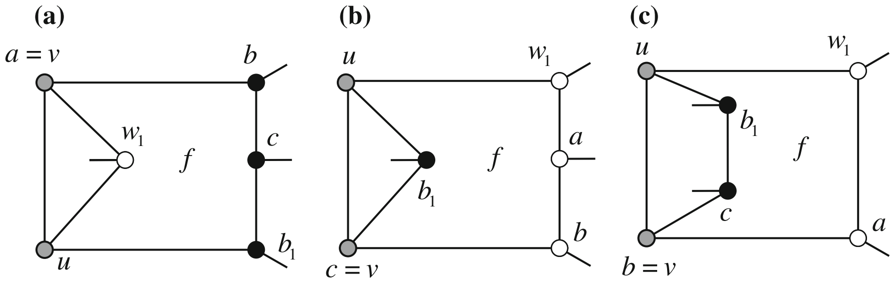
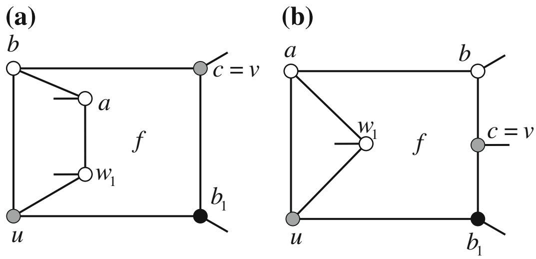


Fig. 3 The illustration for Claim 3 in the proof of Theorem 2.2

Fig. 4 The two cases : **a** u is adjacent to b; and **b** u is adjacent to a



by the fact that u is not adjacent to b or a. Denote by $b_1ux_1a'b'c'b_1$ the boundary of f_1 along the clockwise direction. If $v = a'$, then the four vertices x_1, b, b_1 and b' are pairwise different and they are the neighbors of v, contradicting the 3-regularity of G. If $v = b'$, then $b = a'$ and $c' \in V(H_2)$ (see Fig. 5a). However, in this case we obtain a 3-length cycle $b_1c'vb_1$, contradicting Lemma 2.1 (iii). If $v = c'$, then the vertex b_1 is incident with exactly two faces, which is also a contradiction. If x_1 belongs to $V(H_2)$, then x_1, u, w_1 must be contained in the same hexagon (say f_2) by Claim 1. Denote by $c''w_1ux_1a''b''c''$ the boundary of f_2 such that a'' and c'' are the neighbors of x_1 and w_1, respectively. Since v is not adjacent to w_1, $v \neq c''$. If $v = b''$, then $b_1 = a''$ by the 3-regularity of G and the fact that w_1 is not adjacent to b (see Fig. 5b). However, in this case we obtain a 3-length cycle $C = ub_1x_1u$ contradicting Lemma 2.1 (iii). If $v = a''$, that is, x_1 is adjacent to v, then $b = b''$ since the neighbors of v are x_1, b_1 and b and there are no edges between $V(H_1)$ and $V(H_2)$ (see Fig. 5c). Furthermore, $c'' \neq a$. Now we obtain two 4-length cycles C_1 (with the boundary $w_1abc''w_1$) and C_2 (with the boundary $x_1ub_1vx_1$) (see Fig. 5c), then $G \cong T_n$ for some $n \geq 1$ by Lemma 2.1 (ii). A similar discussion for $v = b$ and $v = a$ will bring us to the conclusion that the graph satisfying the conditions does not exist or it is isomorphic to the graph T_n for some $n \geq 1$. □

Theorem 2.3 *For a (3,6)-fullerene with connectivity 2, each hexagon is not resonant.*

Proof Since $G \cong T_n$ for some $n \geq 1$ by Theorem 2.2, the deletion of any hexagon in Fig. 1 will give rise to two odd components. So each hexagon is not resonant. □

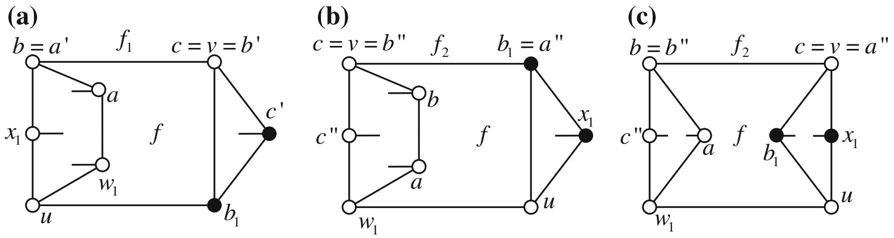


Fig. 5 The illustration in the proof of Theorem 2.2

Corollary 2.4 *Any (3,6)-fullerene with connectivity 2 is not 1-resonant.*

3 (3,6)-fullerenes with connectivity 3

In this section we will show that every hexagon of a (3,6)-fullerene with connectivity 3 except for one graph is resonant. To this end we introduce some terminologies. A graph G is *factor-critical* if $G - v$ has a perfect matching for every vertex $v \in V(G)$. It is known that every factor-critical graph has an odd number of vertices and is 2-edge connected unless it is trivial. Here a factor-critical graph is *trivial* if it consists of a single vertex. We call a vertex set $S \subseteq V(G)$ *matchable* to $G - S$ if the (bipartite) graph H_s which arises from G by contracting the components $c \in \mathcal{C}_{G-S}$ to single vertices and deleting all the edges inside S, contains a matching of S, where $\mathcal{C}_{G-S}$ are the components of $G - S$. The following theorem [5, Theorem 2.2.3], may be viewed as a strengthening of Tutte's 1-factor theorem [23]:

Theorem 3.1 *Every graph G with vertex set $V(G)$ and edge set $E(G)$ contains a vertex set $S \subseteq V(G)$ with the following two properties:*

(i) *S is matchable to $G - S$,*
(ii) *Every component of $G - S$ is factor-critical.*

Furthermore, given any such set S, G has a perfect matching $\iff |S| = |\mathcal{C}_{G-S}|$.

Lemma 3.2 *Let G be a (3,6)-fullerene graph with connectivity 3 which is different from K_4, then the four triangles of G are pairwise nonadjacent.*

Proof Obviously, the four triangles of K_4 are pairwise adjacent. Suppose to the contrary that there exist two triangles in G which are adjacent, then we can obtain a 2-vertex cut, contradicting the 3-connectivity of G. □

An *edge-cut* of a connected graph G is a set of edges $\mathcal{C} \subset E(G)$ such that $G - \mathcal{C}$ is disconnected. A graph G is *cyclically k-edge-connected* if G cannot be separated into two components, each containing a cycle, by removing less than k edges. The *cyclical-edge-connectivity* of G is the greatest integer k such that G is cyclically k-edge-connected. T. Došlić [6] proved that the cyclical-edge-connectivity of (3,6)-fullerenes with connectivity 3 equals 3. There are at least 4 cyclic 3-edge-cuts—formed by the edges pointing outwards of each triangular face. There are also cyclic 6-edge-cuts formed by the edges pointing outwards of each hexagonal faces. These cyclic 3- and 6-edge-cuts are called *trivial*.

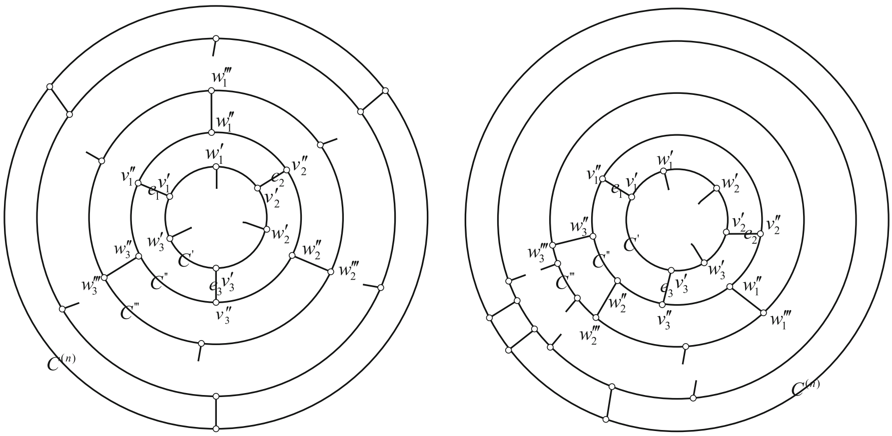


Fig. 6 The only two cases for w_1', w_2', w_3' on the distribution of C'

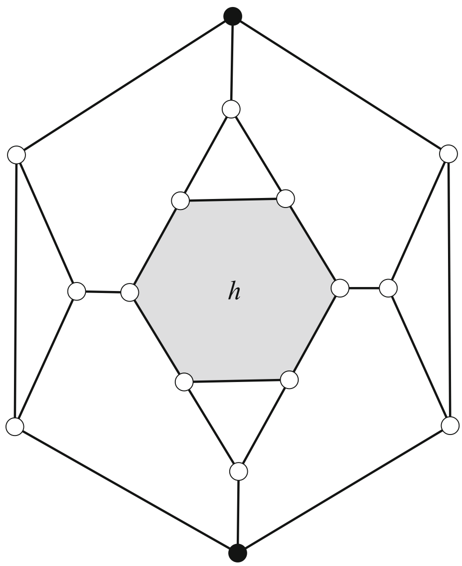
Lemma 3.3 *Every cyclic 3-edge-cut of a (3,6)-fullerene with connectivity 3 is trivial.*

Proof Let G be a (3,6)-fullerene and $C_1 = \{e_1, e_2, e_3\}$ a cyclic 3-edge-cut in G whose deletion separates G into two components, G' and G'', each containing a cycle. Denote the endpoints of e_i in G' and G'' by v_i' and v_i'', respectively, for $i = 1, 2, 3$. Because of 3-connectedness and 3-regularity of G, there are two cycles, C' and C'', such that every edge e_i has one endpoint, say v_i', on C', the other endpoint, v_i'', on C'', and no other edges connects C' with C'' (see Fig. 6). Namely, each of graphs G' and G'' is 2-connected, and in each of them there is only one possible face that is not a face of G. The cycles C' and C'' are exactly the boundary cycles of these exceptional faces in G' and G'', respectively.

To prove the lemma, it suffices to show that G' or G'' is a triangle. That is, there is no additional vertices on C' or C''. Suppose to the contrary that there are k' and k'' additional vertices on C' and C'', respectively. Since G is 3-regular and 3-connected, k' (and k'') must be at least 3. Thus, $k' + k'' \geq 6$. On the other hand, $k' + k'' \leq 6$ because it is impossible to place more than 6 additional vertices on C' and C'', otherwise, there will be at least one face of G with more than 6 edges. So $k' = k'' = 3$.

Denote by w_1', w_2', w_3' the three additional vertices on C' (and w_1'', w_2'', w_3'' on C''). That is, there are exactly six vertices on C' (and C''). Let $G_1' = G' \cup C'' \cup \{e_1, e_2, e_3\}$. This subgraph has three vertices w_1'', w_2'', w_3'' of degree 2 and all other vertices of degree 3. Because of 3-regularity of G, there are three vertices in $G - G_1'$, say w_1''', w_2''', w_3''', which are adjacent with w_1'', w_2'', w_3'', respectively. That is, the edge set $C_2 = \{w_1''w_1''', w_2''w_2''', w_3''w_3'''\}$ separates G into G_1' and $G - G_1'$. Furthermore, the three vertices w_1''', w_2''' and w_3''' are pairwise different by the 3-connectedness of G and Lemma 3.2. So G_1' (respectively, $G - G_1'$) has minimum degree two, thus, each contains a cycle and the edge set C_2 forms a cyclic 3-edge-cut in G. In particular, there exists a cycle C''' in $G - G_1'$ such that C''' is the only one possible boundary cycle that is not a hexagon or a triangle, and no other edges connects C'' with C''' except C_2, and there are precisely six vertices on C''' (see Fig. 6a and b). Using the same approach to

Fig. 7 The (3,6)-fullerene G_2 without a resonant hexagon



the cyclic 3-edge-cut C_2, we have a series of cyclic 3-edge-cuts $C_2, C_3, \ldots, C_n, \ldots$, and the process will be going on, which is impossible. It follows that $k' = 0$ or $k'' = 0$, that is, G' or G'' is a triangle. So the lemma holds. □

Now we state our main result as follows:

Theorem 3.4 *Every hexagon of a (3,6)-fullerene with connectivity 3 except for the graph G_2 (see* Fig. 7*) is resonant.*

Proof First we show that each hexagon of G_2 is not resonant. By the symmetry, it suffices to consider an arbitrary hexagon. Let h be the grey hexagon in Fig. 7. Then the two black vertices of $G_2 - h$ form a vertex set S such that $(G_2 - h) - S$ contains four factor-critical components. By Theorem 3.1, h is not resonant.

Now let G be a (3,6)-fullerene with connectivity 3 which is different from G_2, and h be a hexagon in G. Suppose $G - h$ does not have a perfect matching. Then by Theorem 3.1 there exists an $S \subset V(G-h)$ such that every component of $(G-h)-S$ is factor-critical and $|\mathcal{C}_{G-h-S}| \geq |S|+2$ by parity, i.e. $|S| \leq |\mathcal{C}_{G-h-S}| - 2$, where $\mathcal{C}_{G-h-S}$ are the factor-critical components of $G-h-S$. Since G is 3-regular, S sends out at most $3|S| \leq 3|\mathcal{C}_{G-h-S}| - 6$ edges.

Let $\mathcal{C}_{G-h-S} = \{F_1, F_2, F_3, \ldots, F_k\}$, where $k = |\mathcal{C}_{G-h-S}|$. Because G has no cut-edge, every $F_i (i = 1, 2, \ldots, k)$ sends out odd number edges, hence at least three edges, to $h \cup S$. So $\bigcup_{i=1}^{k} F_i$ sends out at least $3|\mathcal{C}_{G-h-S}|$ edges to $h \cup S$. Since h is a hexagon, $h \cup S$ sends out at most $6 + 3|S| \leq 3|\mathcal{C}_{G-h-S}|$ edges to $\bigcup_{i=1}^{k} F_i$. That is, $\bigcup_{i=1}^{k} F_i$ receives at most $3|\mathcal{C}_{G-h-S}|$ edges from $h \cup S$. Hence there are precisely $3|\mathcal{C}_{G-h-S}|$ edges between $h \cup S$ and $\bigcup_{i=1}^{k} F_i$, and S is an independent set, and every F_i sends out exactly three edges, and there are no edges between h and S.

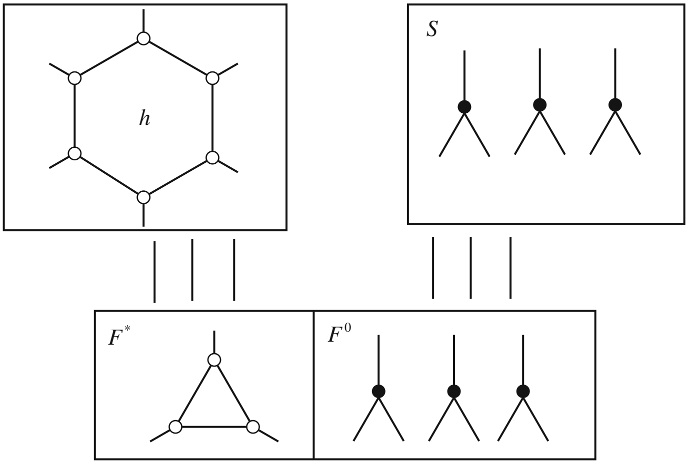


Fig. 8 The partition of $V(G)$ into h, S, F^* and F^0

We denote the subset of non-trivial factor-critical components of $G - h - S$ by $\mathcal{C}^*_{G-h-S}$. The union of the vertex sets of the components of $\mathcal{C}_{G-h-S}$ and $\mathcal{C}^*_{G-h-S}$ is denoted by F and F^*, respectively, and we set $F^0 = F - F^*$ (see Fig. 8).

Claim 1 Every non-trivial factor-critical components of $G - h - S$ is a triangle.

Proof Since every non-trivial factor-critical components of $G-h-S$ sends out exactly three edges which form a cyclic 3-edge-cut, it is a triangle by Lemma 3.3. □

By the Claim, either $\mathcal{C}_{G-h-S}$ is an independent set or it contains at least one triangle. The following lemma is the core of our argument.

Lemma 3.5 *Assume that a, b are adjacent vertices of h and f_1 is the face of G adjacent to h and whose boundary includes the edge ab. Let a', b' be the adjacent vertices of a and b, respectively, not in h. Then f_1 is either a triangle face or a hexagonal face with exactly one of $\{a', b'\}$ belonging to F^* and the other to F^0.*

Proof Suppose f_1 is a hexagonal face. Then the boundary is $a'abb'xya'$, where $x, y \in V(G)$. Since a' and b' belong neither to h nor to S, we have $a', b' \in F^0 \cup F^*$. If both a' and b' belong to F^0, then x and y must be contained in the same hexagon h by the fact that $E(S \cup V(h)) = E(V(h))$, which is not possible since it is easy to find a vertex cut of size at most two in G, contradicting the 3-connectedness of G. If both a' and b' belong to F^*, then we obtain a non-trivial factor-critical component of $G - h - S$ containing at least four vertices b', x, y, a', contradicting Claim 1. Therefore, one of a', b' belongs to F^* and the other to F^0. □

We shall now use Lemma 3.5 to conclude the analysis. Label clockwise the vertices of h by $v_1, v_2, \ldots, v_6$. Let $f_1, f_2, \ldots, f_6$ be the six faces in G adjacent to h and whose boundaries include the edges $v_1v_2, v_2v_3, v_3v_4, \ldots, v_6v_1$, respectively. By Lemma 3.2, at least one of $f_1, f_2, \ldots, f_6$ is a hexagonal face, say f_1. Denote by $v_1v_2v_{10}v_9v_8v_7v_1$

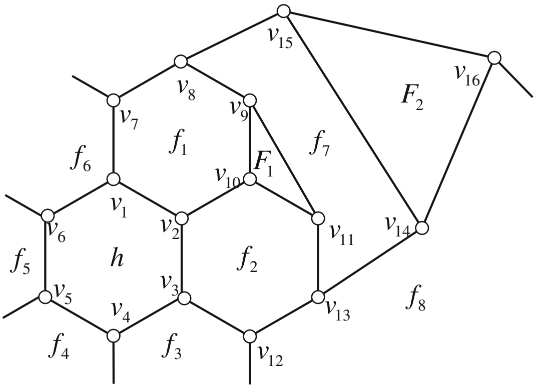


Fig. 9 An illustration to the final argument in the proof of Theorem 3.4 (the case when f_1 is a hexagon and $v_{10} \in F^*$)

the boundary of f_1 along the anticlockwise direction of f_1. Without lose of generality suppose $v_7 \in F^0$ and $v_{10} \in F^*$ by Lemma 3.5. Then both v_{10} and v_9 are contained in a triangle (say F_1) by Claim 1. Since v_8 belongs neither to F nor to h, we have $v_8 \in S$. Let v_{11} be the common neighbor of v_9 and v_{10} (see Fig. 9). Then the four vertices v_3, v_2, v_{10}, v_{11} must be contained in the same hexagon $f_2 = v_2v_3v_{12}v_{13}v_{11}v_{10}v_2$ along the anticlockwise direction. Similarly, $v_{12} \in F^0$ and $v_{13} \in S$. Again we obtain the four vertices v_8, v_9, v_{11}, v_{13} that must be contained in the same hexagonal face (say f_7). Let $v_8v_9v_{11}v_{13}v_{14}v_{15}v_8$ be its boundary along the anticlockwise direction of f_7 (see Fig. 9). Since both v_8 and v_{13} belong to S, v_{14} and v_{15} must be contained in F^* by the fact that $E(F^* \cup F^0) = E(F^*)$. That is, v_{14} and v_{15} must be contained in a triangle (say F_2) by Claim 1.

Denote by $v_{15}v_{14}v_{16}v_{15}$ the boundary of F_2. Then there exist four vertices $v_{12}, v_{13}, v_{14}, v_{16}$ that must be contained in the same hexagonal face (say f_8). Moreover, since v_{12} and v_{16} belong to F and $E(S \cup V(h)) = E(V(h))$, both of v_{12} and v_{16} must be adjacent to $V(h)$ in order to form the hexagonal face f_8. If v_{12} is adjacent to v_5, then v_{16} must be adjacent to v_6 by the planarity of G, which is impossible since we obtain a vertex cut of size one. Therefore, v_{12} and v_{16} must be adjacent to v_4 and v_5, respectively. Then the remaining two vertices v_6 and v_7 must be adjacent, otherwise, there exists a vertex cut of size two, contradicting the fact that G is 3-connected. However, the graph we obtained above is isomorphic to the graph G_2. This contradiction to the assumption completes the proof of Theorem 3.4. □

To consider the k-resonance ($k \geq 2$) of (3,6)-fullerenes with connectivity 3, the following lemma is presented.

Lemma 3.6 *Let G be a (3,6)-fullerene with connectivity 3 which is different from K_4, and F_1 be one of the four triangles in G. Then the three faces adjacent to F_1 are all hexagons and pairwise different and both of them intersect at exactly one edge.*

Proof The first assertion can be easily acquired by Lemma 3.2. If two of the three hexagonal faces are the same, then there exists a vertex incident with exactly two faces, which is impossible. If two of the three hexagonal faces intersect at more than one edge, then we can find a vertex cut of size one, contradicting the 3-connectedness of G. □

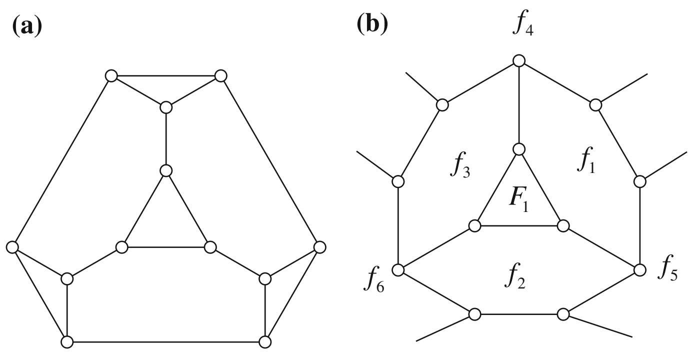


Fig. 10 Illustration for the proof of Theorem 3.7

Theorem 3.7 *For a (3,6)-fullerene graph with connectivity 3 except for the graphs K_4 and G_3 (see* Fig. 10*a), there exist a pair of disjoint hexagons not forming a sextet pattern.*

Proof Note if there is no a pair of disjoint hexagons in G, then G is isomorphic to K_4 (the case when there exist two adjacent triangles) or G_3 (see Fig. 10a), the case when the four triangles in G are pairwise nonadjacent).

Now let G be a (3,6)-fullerene different from K_4 and G_3, and F_1 be one of the four triangles in G. By Lemma 3.6, the three hexagonal faces f_1, f_2, f_3 adjacent to F_1 are pairwise different and both of them intersect at exactly one edge. Since G is different from G_3, at least one of the faces f_4, f_5, f_6 of G (say f_4) is a hexagonal face (see Fig. 10b). Moreover, f_4 and f_2 are disjoint. It is easy to see that $\mathcal{H} = \{f_2, f_4\}$ is not a sextet pattern. □

Corollary 3.8 *A (3,6)-fullerene graph G is k-resonant ($k \geq 2$) if and only if G is isomorphic to K_4 or G_3.*

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