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The isolated-pentagon rule and nice substructures in fullerenes*

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Abstract

After fullerenes were discovered, Kroto in 1987 proposed first the isolated-pentagon rule (IPR): the most stable fullerenes are those in which no two pentagons share an edge, that is, each pentagon is completely surrounded by hexagons. To now the structures of the synthesized and isolated (neutral) fullerenes meet this rule. The IPR can be justified from local strain in geometry and π-electronic resonance energy of fullerenes. If two pentagons abut in a fullerene, a 8-circuit along the perimeter of the pentalene (a pair of abutting pentagons) occurs. This paper confirms that such a 8-circuit is always a conjugated cycle of the fullerene in a graph-theoretical approach. Since conjugated circuits of length 8 destabilize the molecule in conjugated circuit theory, this result gives a basis for the IPR in π-electronic resonance. We also prove that each 6-circuit (hexagon) and each 10-circuit along the perimeter of a pair of abutting hexagons are conjugated. Two such types of conjugated circuit satisfy the $(4n + 2)$-rule, and thus stabilise the molecule.

Keywords: Fullerene, patch, stability, isolated pentagon rule, Kekulé structure, conjugated cycle, cyclic edge-cut.

Math. Subj. Class.: 05C70, 05C10, 92E10

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1 Introduction

The *fullerenes* are closed carbon-cage molecules such that every carbon atom has bonds to three other atoms, and the length of each carbon ring is either 5 or 6. Ever since the first fullerene, Buckministerfullerene C_{60}, was discovered by Kroto et al. in 1985 [15], the stabilities of fullerenes have attracted many theorist's attentions. The simple Hückel molecular orbital model that predicts reliably the relative stabilities of planar aromatic hydrocarbons is not generally found to work so well for fullerenes. Kroto [14] in 1987 proposed first the isolated-pentagon rule (IPR): the most stable fullerenes are those in which no two pentagons share an edge, that is, each pentagon is completely surrounded by hexagons. Schmalz et al. [23] gave a more theoretical discussion of the rule in support of the fullerene hypothesis. Indeed the structures of the synthesized and isolated fullerenes meet this rule. The IPR can be justified from local strain and π-electronic resonance of fullerenes; for details, also see a book due to Fowler and Manolopoulos [7]. Pentagon adjacency leads to higher local curvature of the molecule surface and increases the strain energy. On the other hand, according to Hückel $(4n+2)$-rule, conjugated circuits of length $6, 10, 14, \ldots$ stabilize the molecule, whereas conjugated circuits of length $4, 8, 12, \ldots$ destabilize the molecule. Here a conjugated circuit is a cycle of alternating single and double bonds within a Kekulé structure. If two pentagons abut in a fullerene, the conjugated or resonant 8-circuit along the perimeter of the pentalene may occur, and this leads to resonance destabilization [22]. This is an interpretation of IPR in π-electronic resonation stabilization. However, a problem occurs: In a fullerene, is every 8-length circuit conjugated? To now we have not seen any definite answer to this problem in mathematics. In this article we investigate nice patches of a fullerene by applying some small cyclic edge-cuts of graphs and present a positive answer to the above problem (a patch of a fullerene is nice if its Kekulé structure can be extended to a Kekulé structure of the entire fullerene). As immediate consequences of our main theorems, we have that every 8-length circuit of a fullerene surrounds a pentalene (a pair of abutting pentagons) and is conjugated or alternating with respect to a Kekulé structure (see Corollary 3.4). This confirms the destabilization of any pentalene as a nice substructure to the entire fullerene and thus gives a mathematical support for the IPR of fullerenes. Furthermore we also show that in a fullerene every hexagon is a conjugated 6-circuit (see Corollary 3.3) and the boundary along a naphthalene (i.e. a pair of abutting hexagons) is a conjugated 10-circuit (see Corollary 4.2). The former has already been proved (see [26]). In conjugated circuit theory [10, 19, 20], conjugated 6-circuits and 10-circuits contribute stabilizations of fullerenes and the small conjugated circuits have the greatest effects (positive and negative) on stability. For recent discussions on the IPR of fullerenes about steric strain factor and π-electronic resonance factor, see [1, 2, 8, 13, 21]. For mathematical aspects of fullerenes, see a recent survey [3].

2 Preliminary

To obtain the above end we now start our arguments in a graph-theoretical approach. As a molecular graph of a fullerene, a *fullerene graph* is a 3-connected planar cubic graph with only pentagonal and hexagonal faces. It is well known that a fullerene graph on n vertices exists for every even $n \geq 20$ except $n = 22$ [9]. By Euler's polyhedron formula, every fullerene graph with n vertices has exactly 12 pentagonal faces and $(n/2 - 10)$ hexagonal faces.

Let G be a graph with vertex-set $V(G)$ and edge-set $E(G)$. An edge set M of a graph

G is called a *matching* if no two edges in M have a common endvertex. A matching M of G is *perfect* if every vertex of G is incident with one edge in M. In organic molecular graphs, perfect matchings correspond to Kekulé structures, playing an important role in analysis of the resonance energy and stability of polycyclic aromatic hydrocarbons.

The following classical theorem is Tutte's 1-factor theorem on the existence of perfect matching of a graph [24]. For detailed monograph on matching theory, see Lovász and Plummer [17].

Theorem 2.1. *A graph G has a perfect matching if and only if* $\mathrm{odd}(G-S) \leq |S|$ *for each* $S \subseteq V(G)$*, where* $\mathrm{odd}(G-S)$ *denotes the number of odd components in subgraph* $G-S$.

Subgraph G' of a graph G is called *nice* if $G - V(G')$ has a perfect matching. In particular, an even cycle C of a graph G is nice if G has a perfect matching M such that C is an M-alternating cycle, i.e. the edges of C alternate in M and $E(G) \setminus M$. A nice even cycle is also called *resonant* or *conjugated* cycle (or circuit) in chemical literature. For convenience, a cycle of length k is said to be a k-cycle or k-circuit.

For nonempty subsets X, Y of $V(G)$, let $[X, Y]$ denote the set of edges of G that each has one end-vertex in X and the other in Y. If $\overline{X} = V(G) \setminus X \neq \emptyset$, then $\nabla(X) := [X, \overline{X}]$ is called an *edge-cut* of G, and k-*edge-cut* whenever $|[X, \overline{X}]| = k$. The edges incident with a single vertex form a *trivial* edge-cut. For a subgraph H of G, let $\overline{H} := G - V(H)$. We simply write $\nabla(H)$ for $\nabla(V(H))$.

Lemma 2.2 ([25])**.** *Every* 3*-edge-cut of a fullerene graph is trivial.*

Lemma 2.3 ([25])**.** *Every* 4*-edge-cut of a fullerene graph isolates an edge.*

An edge-cut $S = \nabla(X)$ of G is *cyclic* if at least two components of $G-S$ each contains a cycle. The minimum size of cyclic edge-cuts of G is called *cyclic edge-connectivity* of G, denoted by $c\lambda(G)$.

Theorem 2.4 ([6, 12, 18])**.** *Let F be any fullerene graph. Then* $c\lambda(F) = 5$.

From the definition with the above properties we know that each fullerene graph has the girth 5 (the minimum length of cycles), and each of its 5-cycles and 6-cycles bounds a face. A cyclic k-edge-cut of a graph isolating just a k-cycle will be called *trivial*.

Theorem 2.5 ([12, 16])**.** *A fullerene graph with a non-trivial cyclic* 5*-edge-cut is a nanotube with two disjoint pentacaps (see Figure 1), and each non-trivial cyclic* 5*-edge-cut must be an edge set between two consecutive concentric cycles of length* 10.

A fullerene patch is a 2-connected plane graph with all faces pentagonal or hexagonal except one external face, all internal vertices (not incident with the external face) of degree 3 and those incident with the external face having degree 2 or 3. The cycle bounding the external face is the *boundary* of the patch. We can count the pentagons of a fullerene patch as internal faces as follows.

Lemma 2.6 ([4])**.** *For fullerene patch G, let p_5 denote the number of pentagonal faces other than the external face. Then*

$$p_5 = 6 + k_3 - k_2 = 6 + 2k_3 - l, \tag{2.1}$$

where k_2 and k_3 denote the number of vertices of degree 2 *and* 3 *on the boundary of G, respectively, and l is the boundary length.*

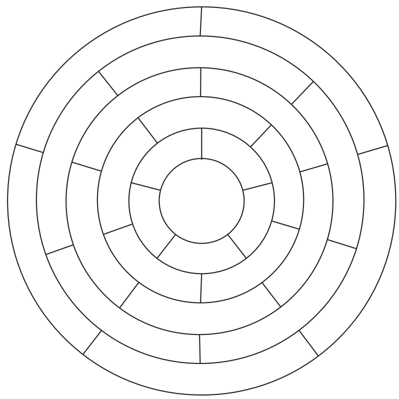

Figure 1: A fullerene with a non-trivial cyclic 5-edge-cut.

For $T \subseteq V(G)$, the induced subgraph of G by T consists of T and all edges whose endvertices are contained in T, denoted by $G[T]$.

In the next two sections we will investigate nice patches of fullerene graphs in cyclic 6-edge-cut and 8-edge-cut cases, respectively.

3 Cyclic 6-edge-cut

We first consider a more general case than fullerene patches.

Theorem 3.1. *Let F_0 be a connected induced subgraph of a fullerene graph F such that interior faces of F_0 exist and each one is a pentagon or hexagon. If F has exactly six edges from F_0 to the outside $\overline{F}_0 = F - V(F_0)$, then F_0 has a perfect matching.*

Proof. Let n_0 and ϵ_0 denote the numbers of vertices and edges of F_0 respectively. Then $3n_0 = 2\epsilon_0 + 6$, which implies that n_0 is even, i.e. F_0 has an even number of vertices.

We will prove that F_0 has a perfect matching by Tutte's theorem. To the contrary suppose that F_0 has no perfect matchings. By Theorem 2.1, there exists a subset $X_0 \subset V(F_0)$ such that

$$\mathrm{odd}(F_0 - X_0) > |X_0|. \tag{3.1}$$

For the sake of convenience, let $\alpha := \mathrm{odd}(F_0 - X_0)$. Since α and $|X_0|$ have the same parity, we have

$$\alpha \geq |X_0| + 2. \tag{3.2}$$

Let $G_1, \ldots, G_\alpha$ and $G_{\alpha+1}, \ldots, G_{\alpha+\beta}$ denote respectively the odd components and the even components of $F_0 - X_0$, where β denotes the number of even components of $F_0 - X_0$. For $i = 1, 2, \ldots, \alpha + \beta$, let m_i denote the number of edges of F_0 which are sent to X_0 from G_i, and γ_i (resp. γ_0) the number of edges of F from G_i (resp. X_0) to $\overline{F}_0$. Since $\nabla(F_0)$ is a 6-edge-cut of F, we have

$$|\nabla(F_0)| = \sum_{i=0}^{\alpha+\beta} \gamma_i = 6. \tag{3.3}$$

Since F is 3-connected, for $i = 1, \ldots, \alpha, \ldots, \alpha + \beta$ we have

$$|\nabla(G_i)| = m_i + \gamma_i \geq 3. \tag{3.4}$$

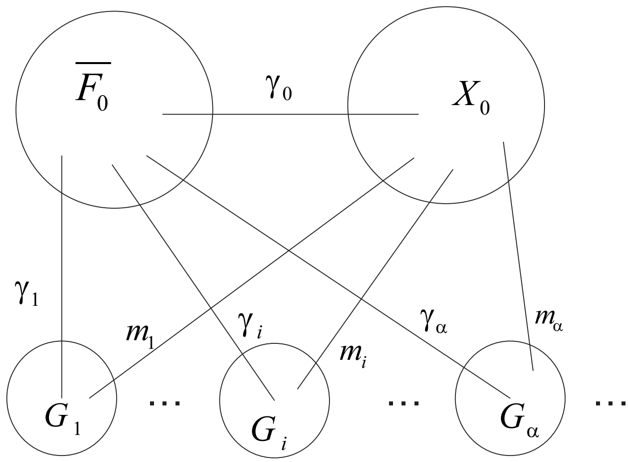

Figure 2: Illustration for the proof of Theorem 3.1.

By taking the number of edges of F from the components G_i to $\overline{F}_0$ and X_0 into account and by using Equation (3.3) and Inequalities (3.2) and (3.4) we have

$$\begin{aligned} 3(\alpha+\beta) &\leq \sum_{i=1}^{\alpha+\beta}(m_i+\gamma_i) \\ &\leq 3|X_0| - \gamma_0 + \sum_{i=1}^{\alpha+\beta}\gamma_i \\ &= 3|X_0| + 6 - 2\gamma_0 \\ &\leq 3\alpha - 2\gamma_0, \end{aligned} \tag{3.5}$$

which implies that $\beta = 0$, $\gamma_0 = 0$ and equalities always hold. Hence $\sum_{i=1}^{\alpha}\gamma_i = 6$, and $\alpha = |X_0| + 2$. Further, the second equality in (3.5) implies that X_0 is an independent set of F_0. The first equality in (3.5) implies that $m_i + \gamma_i = 3$ for each $1 \leq i \leq \alpha$, that is, $\nabla(G_i)$ is a 3-edge-cut of F. So by Lemma 2.2 it is a trivial edge-cut and each G_i is a singleton. Let Y_0 denote the set of all singletons G_i. Then F_0 is a bipartite graph with partite sets X_0 and Y_0.

If F_0 has no vertices of degree one, then F_0 is 2-connected. Otherwise, F_0 has a bridge, the deletion of which results in two components each containing a cycle. So the bridge together with at most three edges in $\nabla(F_0)$ form a cyclic edge-cut, contradicting that $c\lambda(F) = 5$ (Theorem 2.4). Hence F_0 is a fullerene patch. Since $k_2 = |\nabla(F_0)| = 6$, by Lemma 2.6 we have that the number p_5 of pentagons contained in F_0 is equal to the number k_3 of vertices of degree three lying on the boundary of F_0. Since F_0 is bipartite, $k_3 = p_5 = 0$, which implies that F_0 is just a hexagon, contradicting that $\alpha = |Y_0| = |X_0| + 2$.

If F_0 has a vertex x of degree one, let xy be the edge of F_0, and xy_1 and xy_2 be the other two edges in F incident with x. Then $\nabla(F_0 - x) = (\nabla(F_0) \setminus \{xy_1, xy_2\}) \cup \{xy\}$ forms a cyclic 5-edge-cut of F since $F_0 - x$ contains all cycles of F_0 and $\overline{F_0 - x}$ can be obtained from $F - F_0$ by adding a 2-length path y_1xy_2 and contains at least seven pentagons. Since $F_0 - x$ is bipartite, cyclic 5-edge-cut $\nabla(F_0 - x)$ is not trivial, and $F_0 - x$

is always 2-connected from Theorem 2.5. By Lemma 2.6 we have $p_5 = k_3 + 1$ for the fullerene patch $F_0 - x$, which implies that F_0 has at least one pentagon, contradicting that F_0 is bipartite. □

Corollary 3.2. *For each cyclic 6-edge cut E_0 of a fullerene graph F, both components of $F - E_0$ have a perfect matching.*

Proof. It follows that $F - E_0$ has exactly two components from Lemma 2.2 and 3-edge-connectedness of F. Such two components fulfil the conditions of Theorem 3.1 and thus each has a perfect matching. □

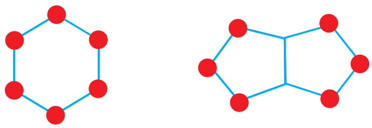

Figure 3: Some nice substructures of fullerene graphs.

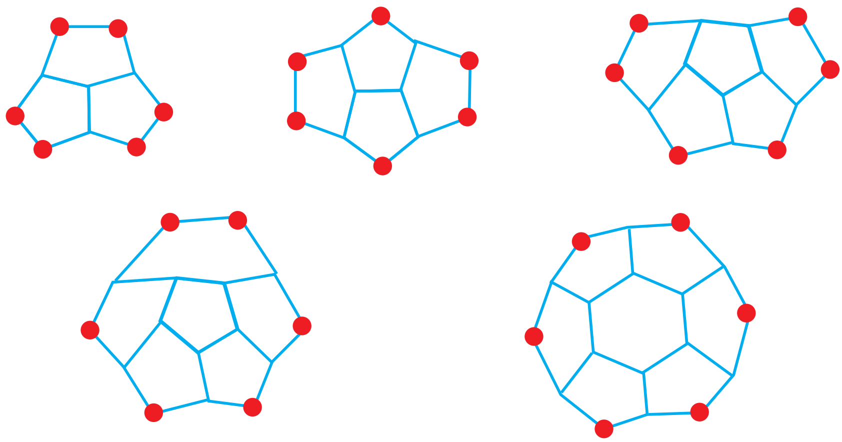

Figure 4: Some nice patches of fullerene graphs with six 2-degree vertices.

From Corollary 3.2 we can find many nice substructures of fullerene graphs, examples of which are shown in Figures 3 and 4. It should be mentioned that the third nice substructure fulvene in Figure 3 has been discovered by Došlić applying 2-extendability of fullerenes [5, 27], and the first one has been proved in investigating k-resonance [26, 11]; see the following.

Corollary 3.3 ([26])**.** *Each hexagon of a fullerene graph is resonant.*

Corollary 3.4. *Each 8-length cycle (if exists) of a fullerene graph bounds a pentalene (a pair of abutting pentagons) and is thus resonant.*

Proof. Let C be a 8-length cycle of a fullerene graph F. If F has an edge e whose endvertices both lie in C but $e \notin E(C)$, then e is called a *chord* of C. If C has no chords, then the eight edges issuing from C can be classified into two edge-cuts of size from 3 to 5, which lie in the interior and the exterior of C respectively. If one is a 3-edge-cut, then Lemma 2.2 implies that it is trivial, and thus a triangle or quadrilateral appear, a contradiction. If both are 4-edge-cuts, then Lemma 2.3 implies that F has only 12 vertices, also a contradiction. So C must have a chord. Further, this chord and C form a pair of 5-length cycles sharing this chord, which must bound pentagonal faces of F by Theorem 2.4. That is, C bounds a pentalene and is resonant from Corollary 3.2. □

4 Cyclic 8-edge-cut

Theorem 4.1. *If E_0 is a cyclic 8-edge-cut of a fullerene graph F and E_0 is a matching, then $F - E_0$ has a perfect matching.*

Proof. There exists a nonempty and proper subset X of vertex set $V(F)$ such that $E_0 = \nabla(X) = [X, \overline{X}]$. Let $F_0 := F[X]$ and $\overline{F}_0 := F[\overline{X}]$. We claim that both F_0 and $\overline{F}_0$ are connected and E_0 is a minimal edge-cut. If not, then one of F_0 and $\overline{F}_0$, say $\overline{F}_0$, is disconnected. Then $\overline{F}_0$ has exactly two components since F is 3-connected. Since E_0 is a matching, F_0 and each component of $\overline{F}_0$ have the minimum degree 2 and contain a cycle. So a cyclic edge-cut of at most four edges occurs in F, a contradiction. So the claim is verified. Hence each of F_0 and $\overline{F}_0$ has exactly one face of size more than six, which has exactly 8 two-degree vertices on its boundary.

We only show that F_0 has a perfect matching (the same for $\overline{F}_0$). If F_0 has a bridge, then it follows that F_0 can be obtained from two pentagons by adding one edge between them by Theorems 2.4 and 2.5. In this case F_0 has a perfect matching. So in the following we always suppose that F_0 is a patch of F. We adopt similar arguments and notations as in the proof of Theorem 3.1 (see Figure 2). It is known that F_0 has an even number of vertices. Suppose to the contrary that F_0 has no perfect matchings. By Tutte's theorem we can choose a *minimal* subset $X_0 \subset V(F_0)$ satisfying $\alpha := \text{odd}(F_0 - X_0) \geq |X_0| + 2$.

Let $G_1, \ldots, G_\alpha$ and $G_{\alpha+1}, \ldots, G_{\alpha+\beta}$ denote respectively the odd components and the even components of $F_0 - X_0$. For $i = 1, 2, \ldots, \alpha + \beta$, let m_i denote the number of edges of F_0 which are sent to X_0 from G_i, and γ_i (resp. γ_0) the number of edges of F from G_i (resp. X_0) to the patch $\overline{F}_0$. By $|\nabla(F_0)| = \sum_{i=0}^{\alpha+\beta} \gamma_i = 8$ and Inequality (3.4), we have

$$\begin{aligned} 3(\alpha+\beta) &\leq \sum_{i=1}^{\alpha+\beta} (m_i + \gamma_i) \\ &\leq 3|X_0| - \gamma_0 + \sum_{i=1}^{\alpha+\beta} \gamma_i \\ &= 3|X_0| + 8 - 2\gamma_0 \\ &\leq 3\alpha + 2 - 2\gamma_0, \end{aligned} \tag{4.1}$$

which implies that $\beta = 0$, $0 \leq \gamma_0 \leq 1$, and $|X_0| + 2 = \alpha$. So the forth equality in Inequality (4.1) holds.

If $\gamma_0 = 1$, then $|[X - X_0, \overline{X}]| = \sum_{i=1}^{\alpha+\beta} \gamma_i = 7$ and all equalities in Inequality (4.1) hold. Like the proof of Theorem 3.1 we have that X_0 is an independent set, $m_i + \gamma_i = 3$ for each $1 \leq i \leq \alpha$ and each G_i is a singleton. Hence F_0 is a bipartite graph. By Lemma 2.6 we have that F_0 has two three-degree vertices on the boundary of F_0. That implies that

F_0 is just the graph obtained by gluing two hexagons along an edge. So F_0 has the same cardinalities of two partite sets, which contradicts that $|X_0| + 2 = \alpha$.

From now on we suppose that $\gamma_0 = 0$. That is, each vertex of X_0 has degree 3 in F_0. We claim that second equality in Inequality (4.1) must hold. Otherwise, $F_0[X_0]$ has exactly one edge, say uv, and the first equality holds, so each G_i is a singleton. Without loss of generality, suppose that y_1 and y_2 are two neighbors of u other than v, and $V(G_1) = \{y_1\}$ and $V(G_2) = \{y_2\}$. Let $X_0' := X_0 \setminus \{u\}$, and $X_1 := \{u, y_1, y_2\}$. Then $G_1' := F_0[X_1]$ is a 3-vertex path obtained by combining G_1 and G_2 with vertex u. Hence $F_0 - X_0'$ has the odd components $G_1', G_3, \dots, G_\alpha$, and $\text{odd}(F_0 - X_0') = \alpha - 1 = |X_0'| + 2$, contradicting the minimality of X_0.

Hence X_0 is an independent set of F_0, and the first inequality is strict. Since for each $1 \le i \le \alpha$, $m_i + \gamma_i$ is always odd, there exists an i_0 such that $m_{i_0} + \gamma_{i_0} = 5$ and $m_i + \gamma_i = 3$ for all $i \ne i_0$. For convenience, we may suppose that $i_0 = 1$. So G_1 is an odd component with at least three vertices and $G_2, \dots, G_\alpha$ are all singletons. Let Y_0 denote the set of all singletons G_i ($2 \le i \le \alpha$). Then $H := (X_0, Y_0)$ is a bipartite graph as the induced subgraph of fullerene graph F.

If G_1 is a tree, then it is a 2-length path, say xyz, since $\nabla(G_1)$ has exactly five edges. For F_0, by Lemma 2.6 we have $p_5 = k_3 - 2$. Since E_0 is a matching, x and z both have neighbors in X_0, so $\gamma_1 \le 3$. The latter implies $\sum_{i=2}^{\alpha} \gamma_i \ge 5$. That is, the boundary of F_0 contains at least 5 two-degree vertices belonging to Y_0.

We assert that $p_5 \le 2$. Since H is bipartite, any pentagon P of F_0 must intersect G_1. If P only intersects a vertex of G_1, say z, then $P - z$ is a path of length 3 in H which connects two vertices of X_0, contradicting that any path between two vertices in the same partite set of a bipartite graph has an even length. Similarly we have that P cannot contain both edges of G_1. If F_0 has two distinct pentagons sharing the same edge of G_1, then one pentagon must have two edges G_1, a contradiction. So the assertion holds.

By the assertion and $p_5 = k_3 - 2$ we have $k_3 \le 4$. This implies that the boundary of F_0 has at most 4 vertices in X_0. Let C be the boundary of F_0. Then $C - V(C) \cap X_0$ has at most $|V(C) \cap X_0|$ components. On the other hand, $C - V(C) \cap X_0$ has all singletons in $V(C) \cap Y_0$ as components. But $|V(C) \cap Y_0| \ge 5$, contradicting $|V(C) \cap X_0| \le 4$.

From now on suppose that G_1 contains a cycle. Then $\nabla(G_1)$ is a cyclic 5-edge-cut of F. By Theorem 2.5 $\nabla(G_1)$ is a matching and G_1 is also a patch (precisely, G_1 is a pentagon or contains a pentacap according as the cyclic 5-edge-cut $\nabla(G_1)$ is trivial or not), so each vertex of H has degree at least two, and each component of H contains a cycle. If H is disconnected, then H has exactly two components H_1 and H_2 since F_0 is 2-edge-connected and $\nabla(G_1)$ has exactly five edges. Further, between G_1 and each H_i has at least two edges. So $\nabla(G_1)$ has two consecutive edges along the boundary of G_1 separately from G_1 to H_1 and H_2. These two edges must be contained in a cycle of length at least 8 bounding a face of F, a contradiction. Hence H is connected.

Since G_1 and $\overline{F}_0$ are two connected subgraphs of F with exactly one face of size more than six, there are two possible cases to be considered.

Case 1. G_1 and $\overline{F}_0$ lie in different faces of H. Suppose that G_1 lies in a bounded face f of H and $\overline{F}_0$ does in the exterior face of H. Then the boundary ∂f of f is a 10-length cycle since 5 neighbors of G_1 in H belong to X_0 and are separated by 5 vertices in Y_0. Hence F is a nanotube with two pentacaps and F_0 has exactly 6 pentagons. By Lemma 2.6 the boundary of F_0 has exactly 8 vertices of degree 3 in F_0. Hence the boundary of F_0 is an alternating cycle of three-degree and two-degree vertices. But in this nanotube there is only

10-length cycle as such boundary of a patch, a contradiction.

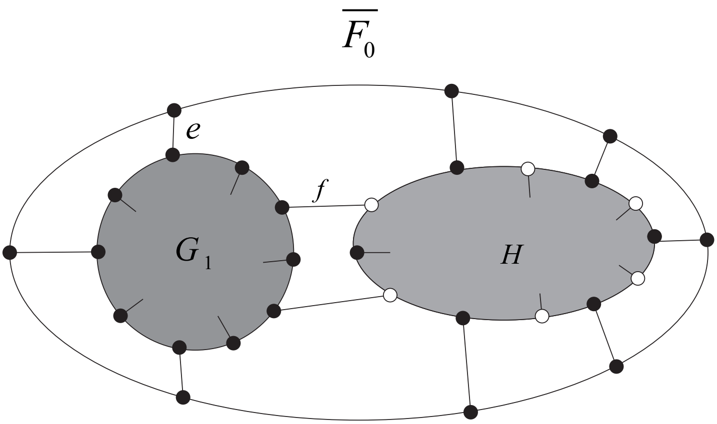

Figure 5: Illustration for Case 2 in the proof of Theorem 4.1 (the vertices in X_0 are colored white and other vertices black).

Case 2. G_1 and $\overline{F}_0$ lie in the exterior face of H. Then the boundary of F_0 is formed by a path P of H and a path P_1 of G_1 and two edges between them. So $0 \leq \gamma_1 \leq 3$, and there are $8 - \gamma_1$ two-degree vertices lying on P, which belong to Y_0 and are thus non-adjacent mutually. So there are at least $7 - \gamma_1$ three-degree vertices in X_0 on P that can separate them. Since the four end-vertices of P and P_1 are all of degree three in F_0, there are at least $11 - \gamma_1$ vertices of degree three of F_0 on the boundary. That is, for F_0, $k_3 \geq 11 - \gamma_1$. On the other hand, if G_1 is a pentagon, then F_0 has at most $5 - \gamma_1$ pentagons, so $k_3 \leq 7 - \gamma_1$ by Lemma 2.6, a contradiction. Otherwise, $\nabla(G_1)$ is a non-trivial cyclic 5-edge-cut and F_0 has exactly 6 pentagons. Hence, by Lemma 2.6 we have that for F_0, $k_3 = 8$. So $\gamma_1 = 3$. Take two consecutive edges e and f of $\nabla(G_1)$ along the boundary of G_1 separately from G_1 to $\overline{F}_0$ and H. Since $\nabla(G_1)$ is a non-trivial cyclic 5-edge-cut, by Theorem 2.5 we have that e and f have non-adjacent end-vertices in G_1. So these two edges belong to a cycle of length at least 7 bounding a face of F (see Figure 5). But this is impossible. □

From Theorem 4.1 we further find many nice substructures of fullerene graphs, which are listed in Figure 6. In particular, the first one is the naphthalene (a pair of abutting hexagons), whose boundary is a resonant cycle of length 10.

Corollary 4.2. *Any adjacent hexagons of a fullerene graph form a nice substructure, and the boundary (*10*-length cycle) is thus resonant.*

However, not all 10-length cycles of fullerene graphs are resonant. For example, see Figure 1. The following corollary gives a criterion for a 10-length cycle of a fullerene graph to be resonant.

Corollary 4.3. *A* 10*-length cycle C of a fullerene graph F is resonant if and only if it bounds either the naphthalene or the second patch in Figure 4.*

Proof. The sufficiency is immediate from Corollaries 3.2 and 4.2. So we only consider the necessity. Suppose that 10-length cycle C of a fullerene graph F is resonant. Let F_0 be

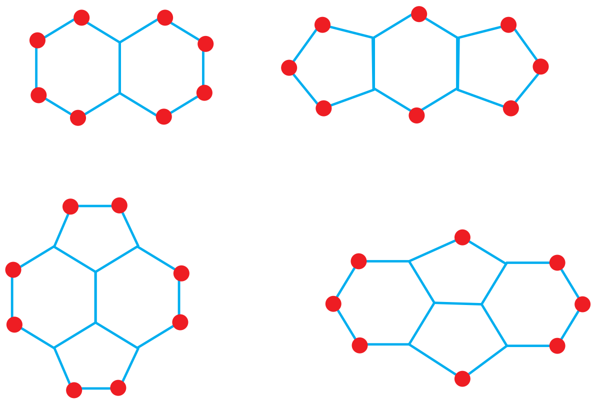

Figure 6: Some nice patches of fullerene graphs with eight 2-degree vertices.

the patch of F bounded by 10-length cycle C with $p_5 \leq 6$. So F_0 has an even number of vertices, and we can have that k_3 and k_2 both are even. By Lemma 2.6 we have $p_5 = 2k_3 - 4$ and $2 \leq k_3 \leq 5$. The possible values of k_3 are 2 and 4. If $k_3 = 2$, then C bounds a pair of adjacent hexagons. If $k_3 = 4$, then F_0 has exactly two vertices in the interior of C which are adjacent by Lemma 2.3. In fact, F_0 is the second patch in Figure 4. □

References

[1] J. Aihara, Bond resonance energy and verification of the isolated pentagon rule, *J. Am. Chem. Soc.* **117** (1995), 4130–4136, doi:10.1021/ja00119a029.

[2] J. Aihara, Graph theory of aromatic stabilization, *Bull. Chem. Soc. Japan* **89** (2016), 1425–1454, doi:10.1246/bcsj.20160237.

[3] V. Andova, F. Kardoš and R. Škrekovski, Mathematical aspects of fullerenes, *Ars Math. Contemp.* **11** (2016), 353–379, doi:10.26493/1855-3974.834.b02.

[4] J. Bornhöft, G. Brinkmann and J. Greinus, Pentagon–hexagon-patches with short boundaries, *European J. Combin.* **24** (2003), 517–529, doi:10.1016/s0195-6698(03)00034-9.

[5] T. Došlić, On some structural properties of fullerene graphs, *J. Math. Chem.* **31** (2002), 187–195, doi:10.1023/a:1016274815398.

[6] T. Došlić, Cyclical edge-connectivity of fullerene graphs and $(k, 6)$-cages, *J. Math. Chem.* **33** (2003), 103–112, doi:10.1023/a:1023299815308.

[7] P. W. Fowler and D. E. Manolopoulos, *An Atlas of Fullerenes*, Clarendon Press, Oxford, 1995.

[8] P. W. Fowler, S. Nikolić, R. De Los Reyes and W. Myrvold, Distributed curvature and stability of fullerenes, *Phys. Chem. Chem. Phys.* **17** (2015), 23257–23264, doi:10.1039/c5cp03643g.

[9] B. Grünbaum and T. S. Motzkin, The number of hexagons and the simplicity of geodesics on certain polyhedra, *Canad. J. Math.* **15** (1963), 744–751, doi:10.4153/cjm-1963-071-3.

[10] W. C. Herndon, Resonance energies of aromatic hydrocarbons: Quantitative test of resonance theory, *J. Am. Chem. Soc.* **95** (1973), 2404–2406, doi:10.1021/ja00788a073.

[11] T. Kaiser, M. Stehlík and R. Škrekovski, On the 2-resonance of fullerenes, *SIAM J. Discrete Math.* **25** (2011), 1737–1745, doi:10.1137/10078699x.

[12] F. Kardoš and R. Škrekovski, Cyclic edge-cuts in fullerene graphs, *J. Math. Chem.* **44** (2008), 121–132, doi:10.1007/s10910-007-9296-9.

[13] A. R. Khamatgalimov and V. I. Kovalenko, Molecular structures of unstable isolated-pentagon-rule fullerenes C_{72}–C_{86}, *Russ. Chem. Rev.* **85** (2016), 836–853, doi:10.1070/rcr4571.

[14] H. W. Kroto, The stability of the fullerenes C_n, with $n = 24, 28, 32, 36, 50, 60$ and 70, *Nature* **329** (1987), 529–531, doi:10.1038/329529a0.

[15] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl and R. E. Smalley, C_{60}: Buckminsterfullerene, *Nature* **318** (1985), 162–163, doi:10.1038/318162a0.

[16] K. Kutnar and D. Marušič, On cyclic edge-connectivity of fullerenes, *Discrete Appl. Math.* **156** (2008), 1661–1669, doi:10.1016/j.dam.2007.08.046.

[17] L. Lovász and M. D. Plummer, *Matching Theory*, AMS Chelsea Publishing, Providence, Rhode Island, 2009, doi:10.1090/chel/367, corrected reprint of the 1986 original.

[18] Z. Qi and H. Zhang, A note on the cyclical edge-connectivity of fullerene graphs, *J. Math. Chem.* **43** (2008), 134–140, doi:10.1007/s10910-006-9185-7.

[19] M. Randić, Conjugated circuits and resonance energies of benzenoid hydrocarbons, *Chem. Phys. Lett.* **38** (1976), 68–70, doi:10.1016/0009-2614(76)80257-6.

[20] M. Randić, Aromaticity and conjugation, *J. Am. Chem. Soc.* **99** (1977), 444–450, doi:10.1021/ja00444a022.

[21] A. Sanz Matías, R. W. A. Havenith, M. Alcamí and A. Ceulemans, Is C_{50} a superaromat? Evidence from electronic structure and ring current calculations, *Phys. Chem. Chem. Phys.* **18** (2016), 11653–11660, doi:10.1039/c5cp04970a.

[22] T. G. Schmalz and D. J. Klein, Fullerene structures, in: W. E. Billups and M. A. Ciufolini (eds.), *Buckminsterfullerenes*, VCH Publishers, New York, chapter 4, pp. 83–101, 1993.

[23] T. G. Schmalz, W. A. Seitz, D. J. Klein and G. E. Hite, Elemental carbon cages, *J. Am. Chem. Soc.* **110** (1988), 1113–1127, doi:10.1021/ja00212a020.

[24] W. T. Tutte, The factorization of linear graphs, *J. London Math. Soc.* **22** (1947), 107–111, doi:10.1112/jlms/s1-22.2.107.

[25] Q. Yang, H. Zhang and Y. Lin, On the anti-forcing number of fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **74** (2015), 673–692, `http://match.pmf.kg.ac.rs/electronic_versions/Match74/n3/match74n3_673-692.pdf`.

[26] D. Ye, Z. Qi and H. Zhang, On k-resonant fullerene graphs, *SIAM J. Discrete Math.* **23** (2009), 1023–1044, doi:10.1137/080712763.

[27] H. Zhang and F. Zhang, New lower bound on the number of perfect matchings in fullerene graphs, *J. Math. Chem.* **30** (2001), 343–347, doi:10.1023/a:1015131912706.