Homeomorphically irreducible spanning trees in fullerene graphs

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1 Introduction

Fullerenes are cubic carbon molecules in which the atoms are arranged on a sphere in pentagons and hexagons. *Fullerene graphs* are 3-connected, 3-regular plane graphs with pentagonal and hexagonal faces, where a *k-regular graph* is a graph with all vertices have degree k and a *plane graph* is a graph drawn on the plane without edge-crossings. Such graphs are suitable models for fullerenes : carbon atoms are represented by vertices of the graph, whereas the edges represent bonds between adjacent atoms. It is known that fullerene graphs satisfy many properties. For example, every fullerene graph is 2-extendable (cf. [5]), contains at least $2^{\frac{n-380}{61}}$ perfect matchings [3] where n is order of the graph, and so on.

In graph theory, it is a fundamental problem deciding a given graph contains a spanning tree with some properties. A *homeomorphically irreducible spanning tree* (or a *HIST*) is a spanning tree with no vertices of degree 2. Recently Hoffmann-Ostenhof, Noguchi and Ozeki [2] found an infinite family of fullerene graphs containing a HIST. In this paper, we consider conditions of fullerene graphs to have a HIST. In particular, we give a necessary and sufficient condition for the existence of a HIST in a fullerene graph (Section 3). Also, we show that there exists an infinite family of fullerene graphs without a HIST (Section 4).

2 Preliminaries

For a graph G, $V(G)$ and $E(G)$ denote the set of vertices and edges of G, respectively. Similarly, $V_i(G)$ denote the subset of $V(G)$ consisting of all degree i vertices in G. Also, $|G|$ and $|E(G)|$ denote the number of vertices and edges of G, respectively. For a vertex $v \in V(G)$, $d_G(v)$ denote the degree of v in G.

2.1 Basic properties of fullerene graphs

Proposition 1 *Let G be a fullerene graph. Then G has $\frac{3}{2}|G|$ edges, exactly twelve pentagonal faces and $\frac{|G|}{2} - 10$ hexagonal faces.*

Proof. Let G be a fullerene graph and let p, q and r be the number of vertices, edges and faces of G, respectively. Let f_5 and f_6 be the number of pentagonal faces and hexagonal faces of G, respectively.

By Euler's formula, we have

$$p - q + r = 2 \tag{2.1}$$

Since G is 3-regular, we have

$$3p = 2q \tag{2.2}$$

Thus we can see that G has $\frac{3}{2}|G|$ edges. Since all faces of G are pentagonal faces or hexagonal faces, we have

$$2q = 5f_5 + 6f_6 = 5r + f_6 \tag{2.3}$$

By combining (2.2) and (2.3), we have

$$5r = 2q - f_6 = 3p - f_6 \tag{2.4}$$

By combining (2.1), (2.2) and (2.4), we have

$$p = 2f_6 + 20 \tag{2.5}$$

and

$$q = 3f_6 + 30 \tag{2.6}$$

By (2.5), we have $f_6 = \frac{p}{2} - 10$. By (2.3) and (2.6), we have $f_5 = 12$. □

A graph G is *cyclically k-edge-connected* if G cannot be separated into two components, each containing a cycle, by deletion of fewer than k edges. Došlić [1] proved that every fullerene graph is cyclically 5-edge-connected. A cyclic edge-cut is called *trivial* if one of the components is a cycle. By the definition, every fullerene graph has a trivial cyclic 5-edge-cut. On the other hand, fullerene graphs containing non-trivial cyclic 5-edge-cut are characterized by Kardoš and Škrekovski [4]. A *pentagonal cap* is a plane graph depicted in Figure 1. In a fullerene graph G, a *hexagonal ring* is a ring consisting of five hexagonal faces such that in each hexagon in the ring there exists a vertex having a neighbor inside this ring, and a vertex having a neighbor outside this ring. Let G_k denote a fullerene graph with the structure that two pentagonal caps are joined by k layers of hexagonal rings.

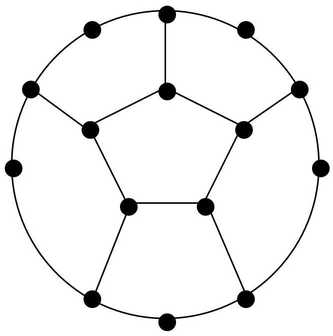

図 1: A pentagonal cap.

Theorem A (Kardoš and Škrekovski [4]) *A fullerene graph G has a non-trivial cyclic 5-edge-cuts if and only if G is isomorphic to G_k for some integer $k \geq 1$.*

2.2 Properties of HISTs in fullerene graphs

First, we introduce a proposition for trees consisting of degree 1 and 3 vertices.

Proposition 2 *Let T be a tree each of whose vertex is degree 1 or 3. Let t_1 and t_3 be the number of vertices of T with degree 1 and 3, respectively. Then $t_1 = t_3 + 2$, that is $t_1 = \frac{|T|}{2} + 1$ and $t_3 = \frac{|T|}{2} - 1$.*

Proof. Let q be the number of edges of T. Since T is a tree, we have

$$2q = t_1 + 3t_3, \quad q = t_1 + t_3 - 1$$

Thus we have $t_1 = t_3 + 2$. □

If a 3-regular graph has a HIST H, then H consists of vertices with degree 1 or 3. Thus, by Proposition 2, we can see the following.

Proposition 3 *Let G be a fullerene graph of order n. Then G has a HIST if and only if G has 2-regular graph S of order $m = \frac{n}{2} + 1$ such that $G - E(S)$ is connected (i.e., S is the set of facial cycles of G which are non-separating).*

Proof. If G has a HIST H, then it is obvious that $G - E(H)$ is a 2-regular graph S if we delete all degree 0 vertices. Also, $G - E(S)$ is connected. So, we show that $|S| = \frac{n}{2} + 1$. Since $|H| = n$, $|E(H)| = n - 1$. Also, $|E(G)| = \frac{3}{2}n$, and hence

$$|S| = |E(S)| = |E(G)| - |E(H)| = \frac{3}{2}n - (n-1) = \frac{n}{2} + 1$$

Next we show that if G has 2-regular graph S of order $m = \frac{n}{2} + 1$ such that $G - E(S)$ is connected, then G has a HIST. Let H' be a graph obtained from G by deleting all edges of S. By the assumptions, H' is connected graph consisting of degree 1 and 3 vertices. Thus it suffices to show that H' is a tree. Since $|S| = \frac{n}{2} + 1$, $|E(S)| = \frac{n}{2} + 1$. So, we have

$$|E(H')| = |E(G)| - |E(S)| = \frac{3}{2}n - (\frac{n}{2} + 1) = n - 1$$

Since $|H'| = n$ and H' is connected, H' is a tree. □

For S in Proposition 3, we can show the following.

Proposition 4 *Let G be a fullerene graph of order n with a HIST and let S be 2-regular graph of order $m = \frac{n}{2} + 1$ such that $G - E(S)$ is connected. Then, for any face f in G, there exists at least one edge on the boundary of f which is contained in $E(S)$.*

Proof. By the proof of Proposition 3, we can see that $G - E(S)$ is a HIST of G, and hence $G - E(S)$ has no cycle. □

3 Necessary and sufficient condition of fullerene graphs to have a HIST

Let G be a plane graph and let G^* be a graph obtained from G by the following operations:

1. Put a new vertex v^* in each face f of G.
2. For every edge e of G, connect the vertices v^* by a edge e^* crossing e.

The resulting graph G^* is called a *dual* of G. Note that G^* may have a loop or multiple edges. By the definition, we can see that if G is a fullerene graph, then G^* is a *plane triangulation* (i.e., a plane graph with all faces are triangular faces) without a loop and multiple edges.

Theorem 5 *Let G be a fullerene graph of order n and let G^* be the dual of G. Then G has a HIST if and only if G^* contains a spanning tree T such that*

(i) for each $v \in V_5(G^*)$, $d_T(v)$ is either 1 or 5,

(ii) for each $u \in V_6(G^*)$, $d_T(u)$ is either 1, 2 or 6,

(iii) for any $x, y \in V(T)$ with degree 2, $xy \notin E(T)$,

(iv) for any $x, y \in V(T)$ with $d_T(x) = 2$ and $d_T(y) = 1$, $xy \notin E(T)$.

Proof. First, we show "only if part". Let H be a HIST of G. By Proposition 3, G has a 2-regular graph S of order $m = \frac{n}{2} + 1$ such that $G - E(S) = H$. By the proof of Proposition 3, we can see that every vertex with degree 1 of H is contained in $V(S)$. By Proposition 4, for each face f in G, there exists at least one edge on the boundary of f which is contained in $E(S)$.

Since G^* is a dual of G, G^* contains 12 vertices of degree 5, $\frac{n}{2} - 10$ vertices of degree 6 and $\frac{3}{2}n$ edges. By the definition of the dual, every edge of G^* crosses to exactly one edge of G and vice versa. Let T be the graph obtained from G^* by deleting all edges which are crossing to $E(H)$. Since H is a spanning tree of G, $|E(H)| = n - 1$, and hence

$$|E(T)| = \frac{3}{2}n - (n-1) = \frac{1}{2}n + 1 = |T| - 1$$

Also, T has no cycle (otherwise H is not connected, a contradiction). Consequently, T is a spanning tree of G^*. Thus it suffices to show that T satisfies the conditions (i)-(iv).

(i) We show that $d_T(v) \neq 2, 3, 4$. Suppose not. Then there are five cases depicted in Figure 2. When the case $d_T(v) = 4$, (a) and (c), H is not connected because the strong lines are independent edges in H, a contradiction. When the case (b) and (d), both v_b and v_d are degree 1 vertices of H. However, they are not contained in $V(S)$, a contradiction.

(ii) We show that $d_T(u) \neq 3, 4, 5$. Suppose not. Then there are seven cases depicted in Figure 3. When the case $d_T(v) = 5$, (a) and (d), H is not connected because the strong lines are independent edges in H, a contradiction. When the case (b), (c), (e) and (f), v_b, v_c, v_e and v_f are degree 1 vertices of H. However, they are not contained in $V(S)$, a contradiction.

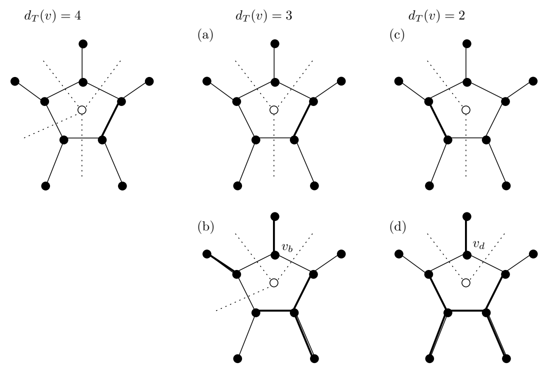

図 2: A part of G (the solid lines) and T (the dot lines).

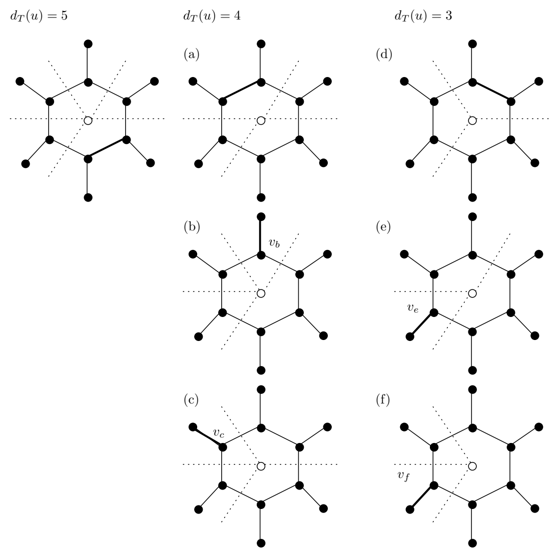

図 3: A part of G (the solid lines) and T (the dot lines).

(iii)-(iv) Let x be a vertex of degree 2 in T and let e_1 and e_2 be edges of T incident to x. By the same arguments in the proof of (i)-(ii), edges e_1 and e_2 are crossing antipodal edges of the hexagonal face of G corresponding to x (otherwise, H contains an independent edge or a degree 1 vertex not contained in $V(S)$, a contradiction). Thus, H contains a vertex of degree 2, a contradiction.

Next we show "if part". So, we prove that if G^* contains spanning tree T satisfying all conditions (i)-(iv), then G has a HIST. Let H be a graph obtained from G by deleting all edges crossing to $E(T)$. Since $|T| = \frac{n}{2}+2$ and T is a tree, $|E(T)| = \frac{n}{2}+1$, and hence

$$E(H) = \frac{3}{2}n - (\frac{n}{2}+1) = n-1$$

Also, H has no cycle (otherwise T is not connected, a contradiction). Therefore, H is a spanning tree of G. So, we show that H has no vertices of degree 2. Suppose not. Then let x be a vertex of H with $d_H(x) = 2$, and let e_1, e_2, e_3 be edges incident to x where $e_1, e_2 \in E(H)$ and $e_3 \notin E(H)$. Let f_1 (resp., f_2) be the face of G incident to e_1 and e_3 (resp., e_2 and e_3). By the conditions (i) and (ii) of T, both f_1 and f_2 are corresponding to vertices of degree 1 or 2 in T. By the conditions (iii) and (iv), we have f_1 and f_2 are corresponding to vertices of degree 1 in T, contrary to that T is a spanning tree of G^*. □

4 Fullerene graphs without a HIST

Theorem 6 *Let G be a fullerene graph. If G has a non-trivial cyclic 5-edge-cuts, then G has no HIST.*

Proof. By Theorem A, it suffices to show that G_k has no HIST for each integer $k \geq 1$. For a contradiction, suppose that G_k has a HIST H for some k. By the construction of G_k,

$$|G_k| = 2 \cdot 15 + 10(k-1) = 10k + 20.$$

By Proposition 3, G_k contains 2-regular subgraph S such that $|S| = \frac{10k+20}{2} + 1 = 5k + 11$ and $G_k - E(S)$ is connected. For a face f of G_k, we call that the *boundary cycle of f is contained in S* if all edges bounding f are contained in S. By Proposition 4, for each face f in G_k, there exists at least one edge on the boundary of f which is contained in $E(S)$. Therefore, for each pentagonal cap of G_k, at least one pentagonal face is contained in S. Let f_i and $f_{k,j}$ be faces depicted in Figure 4 ($f_{2,j}$ are pentagonal faces when $k = 1$).

Suppose that the facial cycle of f_0 is contained in S. Then, for each $i \in \{1,2,3,4,5\}$, facial cycles of f_i and $f_{1,i}$ are not contained in S because $G - E(S)$ is connected. By Proposition 4, for some $j \in \{1,2,3,4,5\}$, facial cycles of $f_{2,j}$ are contained in S. By symmetry, we assume that the facial cycle of $f_{2,1}$ is contained in S. Then, for each $j \in \{2,5\}$, facial cycles of $f_{2,j}$ are not contained in S because $G - E(S)$ is connected. By Proposition 4, at least

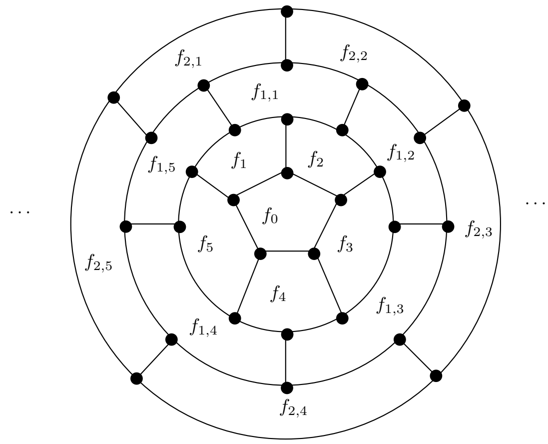

図 4: A pentagonal cap in G_k.

one edge of the boundary cycle of $f_{1,2}$ is contained in S. Also, at least one edge of the boundary cycle of $f_{1,4}$ is contained in S. Therefore, for each $j \in \{3,4\}$, facial cycles of $f_{2,j}$ are contained in S, contrary to that $G - E(S)$ is connected.

Thus the facial cycle of f_0 is not contained in S. By Proposition 4, for some $i \in \{1,2,3,4,5\}$, facial cycles of f_i are contained in S. By symmetry, we assume that the facial cycle of f_1 is contained in S. Then, for each $i \in \{0,2,3,4,5\}$ and $j \in \{1,2,4,5\}$, facial cycles of f_i and $f_{1,j}$ are not contained in S because $G - E(S)$ is connected. Similarly, the facial cycle $f_{2,1}$ is not contained in S. This implies that the facial cycle of $f_{1,3}$ is contained in S by Proposition 4. Therefore, for each $j \in \{2,3,4,5\}$, facial cycles of $f_{2,j}$ are not contained in S.

By the above arguments, the graph obtained from the union of boundary cycles of $f_0, f_2, f_3, f_4, f_5, f_{1,1}$ and $f_{1,5}$ by deleting edges of the union of boundary cycles of f_1 contains a cycle (and hence $G - E(S)$ contains a cycle), contrary to that $G - E(S)$ is a HIST of G. □

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