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# Extremal fullerene graphs with the maximum Clar number☆

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ABSTRACT

A fullerene graph is a cubic 3-connected plane graph with (exactly 12) pentagonal faces and hexagonal faces. Let $F_n$ be a fullerene graph with $n$ vertices. A set $\mathcal{H}$ of mutually disjoint hexagons of $F_n$ is a sextet pattern if $F_n$ has a perfect matching which alternates on and off every hexagon in $\mathcal{H}$. The maximum cardinality of sextet patterns of $F_n$ is the Clar number of $F_n$. It was shown that the Clar number is no more than $\lfloor \frac{n-12}{6} \rfloor$. Many fullerenes with experimental evidence attain the upper bound, for instance, $C_{60}$ and $C_{70}$. In this paper, we characterize extremal fullerene graphs whose Clar numbers equal $\frac{n-12}{6}$. By the characterization, we show that there are precisely 18 fullerene graphs with 60 vertices, including $C_{60}$, achieving the maximum Clar number 8 and we construct all these extremal fullerene graphs.



## 1. Introduction

A *fullerene graph* is a cubic 3-connected plane graph which has exactly 12 pentagonal faces and other hexagonal faces. Fullerene graphs correspond to the fullerene molecule frames in chemistry. Let $F_n$ be a fullerene graph with $n$ vertices. It is well known that $F_n$ exists for any even $n \geq 20$ except $n = 22$ [2,6]. For small $n$, a constructive enumeration of fullerene isomers with $n$ vertices was given [2]. For example, there are 1812 distinct fullerene graphs with 60 vertices including the famous $C_{60}$ synthesized in 1985 by Kroto et al. [14].

Let $F$ be a fullerene graph. A *perfect matching* (Kekulé structure in chemistry) of $F$ is a set $M$ of independent edges such that every vertex of $F$ is incident with an edge in $M$. A cycle of $F$ is $M$-*alternating* (or *conjugated*) if its edges appear alternately in and off $M$. A set $\mathcal{H}$ of mutually disjoint hexagons is called a *sextet pattern* if $F$ has a perfect matching $M$ such that every hexagon in $\mathcal{H}$ is $M$-alternating. So if $\mathcal{H}$ is a sextet pattern of $F$, then $F - \mathcal{H}$ has a perfect matching where $F - \mathcal{H}$ is the subgraph arising from $F$ by deleting all vertices and edges incident with hexagons in $\mathcal{H}$. A maximum sextet pattern is also called a *Clar formula*. The cardinality of a Clar formula is the *Clar number* of $F$, denoted by $c(F)$. In Clar's model [3], a Clar formula is designated by depicting circles within their hexagons (see Fig. 1).

The Clar number is originally defined for benzenoid systems based on the Clar sextet theory [3] and related to Randić conjugated circuit model [17]. It is effective to measure the molecule stability of benzenoid hydrocarbons. For two isomeric benzenoid hydrocarbons, the one with larger Clar number is more stable. Clar numbers of benzenoid hydrocarbons have been investigated and computed in many papers [10,11,13,22,19–21]. Hansen and Zheng [11] introduced an integer linear program to compute the Clar number of benzenoid hydrocarbons. Abeledo and Atkinson [1] showed that relaxing the integer-restrictions in such a program always yields an integral solution.

Up to now there has been no effective method to compute Clar numbers of fullerene graphs. The Clar polynomial and sextet polynomial of $C_{60}$ for counting Clar structures and sextet patterns respectively were computed in [18]. This implies

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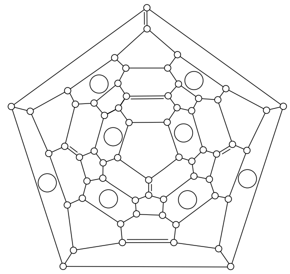

**Fig. 1.** A Clar formula of $C_{60}$.

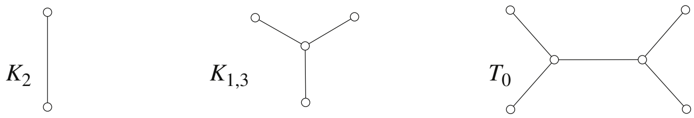


**Fig. 2.** Trees: $K_2$, $K_{1,3}$ and $T_0$.

that $C_{60}$ has 5 Clar formulas and Clar number 8 [5]. In addition, $C_{60}$ has a Fries structure [8], i.e. a Kekulé structure of $C_{60}$ which avoids double bonds in pentagons and has the possibly maximal number of conjugated hexagons ($n/3$). Fullerene graphs with a Fries structure are equivalent to leapfrog fullerenes or Clar type fullerenes [7,15]. The latter means that they have a set of disjoint faces including all vertices, an extension of a fully-Clar structure. Some relationships among the Clar number, the maximum face independent number and Fries number are presented by Graver [9]. A lower bound for the Clar numbers of leapfrog fullerenes with icosahedral symmetry was also given in [9]. The same authors of this paper [23] showed that the Clar number of a fullerene graph with $n$ vertices is no more than $\lfloor \frac{n-12}{6} \rfloor$, for which equality holds for infinitely many fullerene graphs, including $C_{60}$ and $C_{70}$. We would like to mention here that a recent paper of Kardoš et al. [12] obtained a exponentially bound of perfect matching numbers of fullerene graphs. In fact, they applied Four-Color Theorem to show that a fullerene graph with $n \geq 380$ vertices has a sextet pattern with at least $\frac{n-380}{61}$ hexagons.

A fullerene graph $F_n$ is *extremal* if its Clar number $c(F_n) = \frac{n-12}{6}$. In this paper, we characterize the extremal fullerene graphs with at least 60 vertices (Section 3). According to the characterization, we construct all 18 extremal fullerene graphs with 60 vertices, including $C_{60}$ (Section 4). Our result can show that a combination of Clar number and Kekulé count works well in predicting the stability of $C_{60}$.

## 2. Definitions and terminologies

Let $G$ be a plane graph with vertex-set $V(G)$ and edge-set $E(G)$. Let $|G| = |V(G)|$. For a 2-connected plane graph, every face is bounded by a cycle. For convenience, a face is represented by its boundary if unconfused. The boundary of the infinite face of $G$ is also called the boundary of $G$, denoted by $\partial G$. A graph $G$ is *cyclically $k$-edge-connected* if deleting less than $k$ edges from $G$ cannot separate it into two components such that each of them contains at least one cycle. The *cyclic edge-connectivity* of graph $G$, denoted by $c\lambda(G)$, is the maximum integer $k$ such that $G$ is cyclically $k$-edge-connected.

**Lemma 2.1** ([4,16]). *Let $F$ be a fullerene graph. Then $c\lambda(F) = 5$.* □

From now on, let $F$ be a fullerene graph. Let $C$ be a cycle of $F$. Lemma 2.1 implies that the size of $C$ is larger than 4. The subgraph consisting of $C$ together with its interior is called a *fragment*. A *pentagonal fragment* is a fragment with only a pentagonal inner face. For a fragment $B$, all 2-degree vertices of $B$ lie on its boundary.

**Lemma 2.2.** *Let $B$ be a fragment of a fullerene graph $F$ and let $W$ be the set of all 2-degree vertices of $B$. If $0 < |W| \leq 4$, then $T := F - (V(B) \setminus W)$ is a forest and,*

(1) *$T$ is $K_2$ if $|W| = 2$;*
(2) *$T$ is $K_{1,3}$ if $|W| = 3$;*
(3) *$T$ is the union of two $K_2$'s, or a 3-length path, or $T_0$ as shown in Fig. 2 if $|W| = 4$.*

**Proof.** Since $B$ is a fragment, $\partial B$ is a cycle. For every vertex $w \in W$, let $ww_1, ww_2 \in E(\partial B)$. The neighbor of $w$ distinct from $w_1$ and $w_2$ belongs to either $W$ or $V(F - B)$.

If $V(F) = V(B)$, then every vertex in $W$ is adjacent to exactly one 2-degree vertices in $W$. Therefore $|W| = 2$ or $|W| = 4$. If $|W| = 2$, then the two vertices in $W$ are adjacent. Further $T$ is a $K_2$. If $|W| = 4$, then $F$ has two more edges than $B$. If the no vertices in $W$ are adjacent in $B$, then the two edges are disjoint and hence $T$ is a union of two $K_2$. If there are vertices are adjacent, then there are exactly one pair of 2-degree vertices from $W$ adjacent since $F$ contains no 4-length cycle. It follows that $T$ must be a 3-length path consisting of two edges in $E(F) - E(B)$ and one edge in $E(B)$.

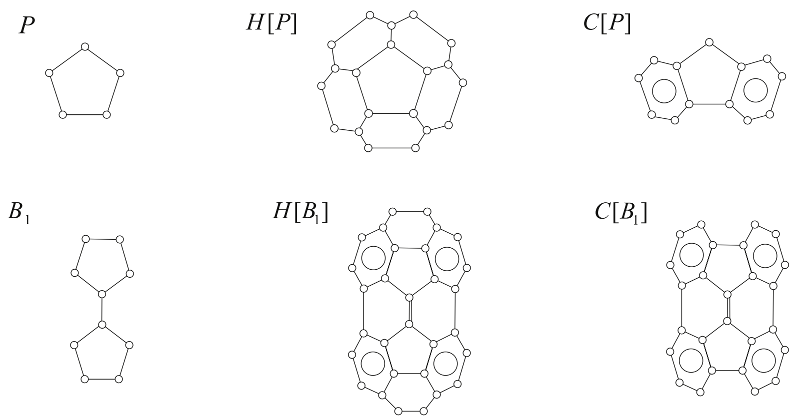


**Fig. 3.** The hexagon extensions and Clar extensions of $P$ and $B_1$.

So suppose $V(F)\setminus V(B)\neq\emptyset$. Let $S$ be a set of the edges joining the vertices in $W$ and their neighbors in $F-B$. Since every vertex in $W$ has at most one neighbor in $F-B$, we have $|S|\leq|W|$. So $S$ separates $B$ from $F-B$. By Lemma 2.1, $F-B$ has no cycles since $|W|\leq 4$.

Suppose to the contrary that $T$ has at least one cycle $C$. Then $C\cap\partial B\neq\emptyset$ since $F-B$ is a forest. We draw $F$ on the plane such that $B$ lies outside of $C$. Then $C$ together with its interior is a subgraph of $T$. We may thus assume that $C$ bounds a face of $F$ within $T$. Since $F$ is cubic, every component of $C\cap\partial B$ is an edge joining two vertices in $W$. By $0<|W|\leq 4$, $C\cap\partial B$ has at most two components.

If $C\cap\partial B$ has two components, then $|W|=4$ and $C$ contains all vertices in $W$. Let $w_1, w_2, w_3, w_4$ be the four vertices in $W$ and let $w_1w_2$ and $w_3w_4$ be the two components of $C\cap B$. Let $w_i'$ be another neighbor of $w_i$ on $\partial B$. Then $\{w_iw_i'|i=1,2,3,4\}$ separates $C$ from $F-C$, contradicting Lemma 2.1.

So suppose $C\cap\partial B$ has only one component $w_1w_2$. Then $C-\{w_1,w_2\}$ is a path in a component $T_1$ of $F-B$. Further $T_1$ has at least $|C|-2$ vertices. If $T_1$ has a 3-degree vertex, then it has at least three leaves. Since every leaf of $T_1$ is adjacent to two vertices in $W$, we have $|W|\geq 6$ which contradicts that $|W|\leq 4$. So $T_1$ is a path. Then $T_1$ has at least $|C|-4$ 2-degree vertices. Hence vertices in $V(T_1)$ have at least $4+|C|-4$ neighbors in $W$. So $|W|\geq 4+|C|-4\geq 5$ which also contradicts that $|W|\leq 4$. So $T$ is a forest.

Let $l$ and $x$ be the number of leaves and the number of components of $T$, respectively. Then $l=|W|\leq 4$. Since $F$ is cubic, $2(|T|-x)=3(|T|-l)+l$. Then $l-2x=|T|-l>0$ since $F-B\neq\emptyset$ and $W\neq\emptyset$. Hence $4\geq l>2x\geq 2$. So we have $x=1$. Hence $T$ is a tree. So if $l=3$, then $T$ is $K_{1,3}$. If $l=4$, then $|T|-l=2$. Hence $T$ is isomorphic to $T_0$. □

For a face $f$ of a connected plane graph, its boundary is a closed walk. For convenience, a face $f$ is often represented by its boundary if unconfused. Note that a pentagon or a hexagon of a fullerene graph $F$ must bound a face since $F$ is cyclic 5-edge-connected [4,23]. Let $G$ be a subgraph of a fullerene graph $F$. A face $f$ of $F$ *adjoins* $G$ if $f$ is not a face of $G$ and $f$ has at least one edge in common with $G$. Now suppose $G$ has no 1-degree vertices. Let $f'$ be a face of $G$ with 2-degree vertices on its boundary. Since $F$ is cubic and 3-connected, $f'$ has at least two 2-degree vertices. A path $P$ on the boundary of $f'$ connecting two 2-degree vertices is *degree-saturated* if $P$ contains no 2-degree vertices of $G$ as intermediate vertices. Since every face of $F$ has a size of at most six, the length of $P$ is no more than five.

**Proposition 2.3.** *Let $G$ be a subgraph of a fullerene graph $F$. Let $f$ be a face of $G$ with* 2*-degree vertices and $P$ be a degree-saturated path of $G$ on the boundary of $f$. Then the length of $P$ is no more than* 5.

Let $f_1, f_2, \ldots, f_k$ be the faces of $F$ adjoining $G$. The subgraph $T[G]:=G\cup(\cup_{i=1}^{k}f_i)$ is called the *territory* of $G$ in $F$. If for every $i\in\{1,2,\ldots,k\}$, the face $f_i$ $(i=1,\ldots,k)$ is a hexagon, the territory is also called a *hexagon extension* of $G$ and is denoted by $H[G]$ (see Fig. 3). A subgraph $G$ is *maximal* in $F$ if $H[G]\subset F$. We are particularly interested in the maximal pentagonal fragments. Denote the number of 2-degree vertices of $G$ by $w(G)$. Let $B$ and $B'$ be two fragments such that $w(B)\geq w(B')$. Let $P$ and $P'$ be two degree-saturated paths of $\partial B$ and $\partial B'$, respectively. Suppose $|P|\leq|P'|$. Let $f$ and $f'$ be two faces adjoining $B$ and $B'$ along $P$ and $P'$, respectively. It is readily seen that $w(B\cup f)\geq w(B'\cup f')$ if $|f|\geq|f'|$. Applying this argument for the territory $T[B]$ and the hexagon extension $H[B]$ of $B$, we immediately have the following proposition.

**Proposition 2.4.** *Let $B$ be a fragment of a fullerene graph $F$ and let $T[B]$ and $H[B]$ be the territory and the hexagon extension of $B$, respectively. Then $w(T[B])\leq w(H[B])$.*

A subgraph (or a set of vertices) $S$ of $F$ *meets* a subgraph $G$ of $F$ if $S\cap G\neq\emptyset$. Let $G-S$ be the subgraph obtained from $G$ by deleting all vertices in $S$ together with all edges incident with them. Let $H[G]$ be the hexagon extension of $G$ and $\mathcal{H}$ be a set of mutually disjoint hexagons of $H[G]$. Let

$$\mathscr{S}(G):=\{\mathcal{H}|\ G-\mathcal{H}\text{ has a matching which covers all remaining 3-degree vertices of }G\}.$$

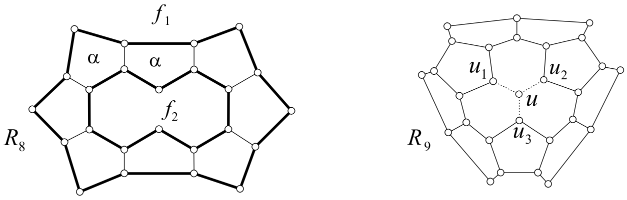


**Fig. 4.** Pentagonal rings: $R_8$ and $R_9$.

For any $\mathcal{H} \in \mathscr{S}(G)$, let $U_{\mathcal{H}}(G) := V(G) \setminus V(\mathcal{H})$. An $\mathcal{H} \in \mathscr{S}(G)$ is called a *Clar set* of $H[G]$ if $|U_{\mathcal{H}}(G)| \leq |U_{\mathcal{H}'}(G)|$ for all $\mathcal{H}' \in \mathscr{S}(G)$. A Clar set $\mathcal{H}$ of $H[G]$ is *normal* if $G - \mathcal{H}$ has a perfect matching. For a fullerene graph $F$, its hexagon extension is itself and a Clar formula of $F$ is a normal Clar set. (See Fig. 3: the hexagons in Clar sets of the hexagon extensions of a pentagon $P$ and $B_1$ are depicted by circles; the Clar set of $H[B_1]$ is normal.)

**Definition 2.5.** Let $G \subseteq F$ and $\mathcal{H}$ be a Clar set of $H[G]$. A *Clar extension* $C[G]$ of $G$ is the subgraph induced by $V(\mathcal{H}) \cup V(G)$. A Clar extension $C[G]$ is *normal* if $\mathcal{H}$ is normal.

The Clar extensions of $P$ and $B_1$ are illustrated in Fig. 3. The Clar extension of a fullerene graph $F$ is itself. Let $\mathcal{H}$ be a Clar formula of $F$ and $U_{\mathcal{H}} := V(F) \setminus V(\mathcal{H})$. The following result is from [23].

**Lemma 2.6** (*[23, Lemma 2]*). *If a subgraph $G$ of a fullerene graph $F$ has at least $k$ pentagons, then $|V(G) \cap U_{\mathcal{H}}| \geq k$.* □

Lemma 2.6 can be generalized as the following result.

**Lemma 2.7.** *Let $G$ be a subgraph of a fullerene graph $F$ with $k$ pentagons and $\mathcal{H}$ be a Clar set of $H[G]$. Then $|U_{\mathcal{H}}(G)| \geq k$.*

**Proof.** Let $G$ be a subgraph of $F$ with $k$ pentagons and $\mathcal{H}$ be a Clar set of $H[G]$. We proceed by induction on $k$. If $k = 1$, $|U_{\mathcal{H}}(G)| \geq 1$ since every pentagon has at least one vertex not in $\mathcal{H}$. So suppose the conclusion holds for smaller $k$.

If $G$ has a 2-degree vertex $v$ in $U_{\mathcal{H}}(G)$, then $G-v$ has at least $k-1$ pentagons. By inductive hypothesis, $|U_{\mathcal{H}}(G-v)| \geq k-1$. So $|U_{\mathcal{H}}(G)| = |U_{\mathcal{H}}(G-v)| + 1 \geq k$ and the lemma holds.

So suppose all vertices in $U_{\mathcal{H}}(G)$ are 3-degree vertices of $G$; that is, $G - V(\mathcal{H})$ has a perfect matching. The proof of this case follows directly from the proof of Lemma 2.6 (Lemma 2 in [23]). □

A subgraph $G$ with $k$ pentagons is *extremal* if $|U_{\mathcal{H}}(G)| = k$ where $\mathcal{H}$ is a Clar set of $H[G]$. Both $P$ and $B_1$ are extremal (see Fig. 3). Note that the every subgraph induced by pentagons of an extremal fullerene graph must be extremal. Hence extremal subgraphs play a key role in characterizing extremal fullerene graphs.

## 3. Extremal fullerene graphs

In this section, we are going to characterize extremal subgraphs induced by pentagons of fullerene graphs and finally establish a characterization of the extremal fullerene graphs with at least 60 vertices.

From now on, let $F_n$ be a fullerene graph with $n$ vertices. A *pentagonal ring* $R_k$ is a subgraph of $F_n$ consisting of $k$ pentagons $P_0, P_1, \ldots, P_{k-1}$ such that $P_i \cap P_j \neq \emptyset$ if and only if $|i-j| = 1$ where $i, j \in \mathbb{Z}_k$ (see Fig. 4). Since $F_n$ has exactly 12 pentagons and $c\lambda(F_n) = 5$, we deduce that $5 \leq k \leq 12$.

**Lemma 3.1.** *If $F_n$ contains a pentagonal ring $R_k$ with $7 \leq k \leq 12$, then $n \leq 52$.*

**Proof.** Let $R_k \subset F_n$ be a pentagonal ring. Let $f_1, f_2 \notin \{P_0, \ldots, P_{k-1}\}$ be two faces of $R_k$. We may assume that $f_1$ is the infinite face. For $i \in \{1, 2\}$, let $x_i$ be the numbers of 2-degree vertices on the boundary of $f_i$.

Let $B$ be the fragment consisting of $f_1$ together with its interior. Let $m_5$ and $m_6$ be the number of pentagons and hexagons of $B$, respectively. By Euler's formula,

$$\nu - e + m_5 + m_6 = 1$$

where $\nu$, $e$ are the vertex number and the edge number of $B$, respectively. On the other hand,

$$2x_1 + 3(\nu - x_1) = 2e = 5m_5 + 6m_6 + 2x_1 + x_2.$$

Hence, $m_5 = 6 + x_2$. Since $m_5 \geq k = x_1 + x_2$, it follows that $x_1 \leq 6$. Since $7 \leq k \leq 12$ and $F$ is 3-connected, $x_2 \geq 2$. It can be verified that $H[B]$ has at most four 2-degree vertices on its boundary. Let $B'$ be the fragment consisting of $f_2$ together with its interior. By Lemma 2.2 and Proposition 2.4, $|V(F - B')| \leq 6 \times 6 - 2 \times 6 + 2 = 26$ since there are at most six faces adjoining $B$ and any two adjacent faces share at least one edge. A similar discussion results in $|V(B')| \leq 26$ since $F$ can be drawn on the plane such that $f_2$ is the infinite face of $R_k$. So $\nu \leq |V(F - B')| + |V(B')| \leq 52$. □

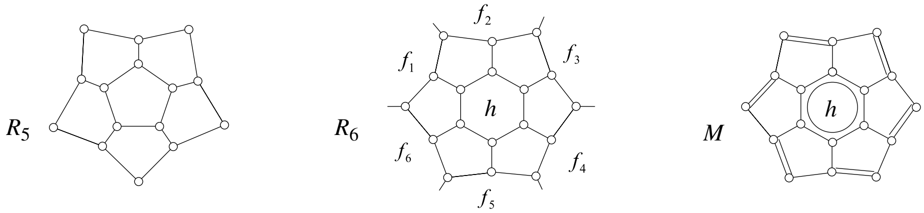


**Fig. 5.** Pentagonal rings $R_5$, $R_6$ and a matching $M$ of $R_6$.

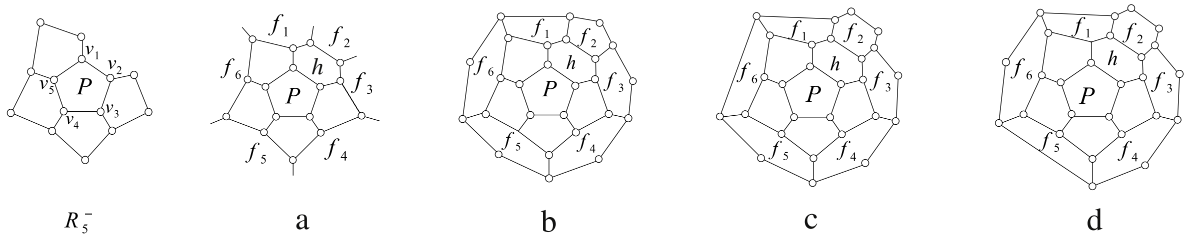


**Fig. 6.** The fragment $R_5^-$ and illustration for the proof of Lemma 3.5.

The following observations show that a subgraph $G$ of $F_n$ (except $F_{24}$) is not extremal if it contains $R_5$ and $R_6$ as subgraphs. Recall that the territory and the hexagon extension of $G$ is denoted by $T[G]$ and $H[G]$, respectively. For a Clar set $\mathcal{H}$ of $H[G]$, define $U_{\mathcal{H}}(G) := V(G) \setminus V(\mathcal{H})$. Let $R_5$ and $R_6$ be the pentagonal rings depicted in Fig. 5.

**Observation 3.2.** *Let $\mathcal{H}$ be a Clar set of $H[R_5]$. Then $|U_{\mathcal{H}}(R_5)| \geq 12$.*

The proof is similar to the proof of Lemma 1 of [23].

**Observation 3.3.** *Let $G$ be a subgraph of a fullerene graph. If $R_5 \subseteq G$, then $G$ is not extremal.*

**Proof.** Suppose to the contrary that $G$ is extremal. Since $R_5 \subseteq G$, we have that $|U_{\mathcal{H}}(G)| \geq |U_{\mathcal{H}}(R_5)| \geq 12$ by Observation 3.2. Hence $G$ has 12 pentagons since $G$ is extremal. Clearly, every pentagon contains at least one vertex in $U_{\mathcal{H}}(G)$ and at least one pentagon does not adjoin $R_5$. So $|U_{\mathcal{H}}(G)| \geq |U_{\mathcal{H}}(R_5)| + 1 = 13$ which contradicts that $G$ is extremal. □

**Observation 3.4.** *Let $G$ be a subgraph of a fullerene graph $F_n$ with $n \neq 24$. If $R_6 \subseteq G$, then $G$ is not extremal.*

**Proof.** Let $\mathcal{H}$ be a Clar set of the hexagon extension $H[G]$ of $G$. Enumerate clockwise the six faces of $F_n$ adjoining $R_6$ as $f_1, \ldots, f_6$ (see Fig. 5). Since $G \subseteq F_n$ ($n \neq 24$), not all $f_i$ ($1 \leq i \leq 6$) are pentagons. Let $r := |\mathcal{H} \cap \{f_1, \ldots, f_6\}|$ and $h$ be the central hexagon of $R_6$.

If $h \notin \mathcal{H}$, then $|U_{\mathcal{H}}(G)| \geq |U_{\mathcal{H}}(R_6)| = 18 - 3r$ since every $f_i$ contains three vertices in $V(R_6)$. If $r \leq 1$, then $G$ is not extremal since $|U_{\mathcal{H}}(G)| \geq 15$ and $G$ has at most 12 pentagons. So $2 \leq r \leq 3$. If $r = 3$, say $f_1, f_3, f_5 \in \mathcal{H}$, then $R_6 - \mathcal{H}$ has no matchings which cover all remaining 3-degree vertices of $R_6$, contradicting that $\mathcal{H}$ is a Clar set. So suppose $r = 2$. Then $G$ has exact 12 pentagons. Over these 12 pentagons, at least two pentagons do not adjoin $R_6$. Since every pentagon contains at least one vertex in $U_{\mathcal{H}}(G)$, it holds that $|U_{\mathcal{H}}(G)| \geq 12 + 1 = 13$. Hence $G$ is not extremal.

So suppose $h \in \mathcal{H}$. Then all 3-degree vertices on $\partial R_6$ of $R_6$ have to match all 2-degree vertices on $\partial R_6$ in $G - \mathcal{H}$ (see Fig. 5, $R_6$ with a matching $M$). So $|U_{\mathcal{H}}(G)| \geq |V(\partial R_6)| = 12$. So suppose $G$ has 12 pentagons. Since $G \subseteq F_n \neq F_{24}$, at least one pentagon in $G$ does not adjoin $R_6$ and has at least one vertex in $U_{\mathcal{H}}(G)$. Immediately, $|U_{\mathcal{H}}(G)| \geq 12 + 1 = 13$. So $G$ is not extremal. □

By the above observations and Lemma 3.1, an extremal fullerene graph with at least 60 vertices does not contain a pentagonal ring as a subgraph. If a connected component of the subgraph induced by pentagons of $F_n$ with $n \geq 60$ is extremal, then it must be a pentagonal fragment.

Let $R_5^-$ be the pentagonal fragment arising from $R_5$ by deleting one 2-degree vertex together with two edges incident with it (see Fig. 6).

**Lemma 3.5.** *Let $G$ be a subgraph of $F_n$ with $n \geq 40$. If $R_5^- \subseteq G$, then $G$ is not extremal.*

**Proof.** Let $G \subseteq F_n$ with $k$ pentagons and $\mathcal{H}$ be a Clar set of $H[G]$. Suppose to the contrary that $G$ is extremal. By Observations 3.3 and 3.4, $R_5 \nsubseteq G$ and $R_6 \nsubseteq G$. Let $P := v_1v_2 \ldots v_5v_1$ be the pentagon of $R_5^-$ meeting all other pentagons of $R_5^-$ as shown in Fig. 5. Let $h$ be the hexagon of $F_n$ adjoining $R_5^-$ along $v_1v_2$ since $R_5 \nsubseteq G$. Let $f_1, f_2, \ldots, f_6$ be the faces of $F_n$ adjoining $R_5^- \cup h$ as shown in Fig. 6(a).

Let $r$ be the number of pentagons in $\{f_1, \ldots, f_6\}$ and $H[R_5^- \cup h]$ be the hexagon extension of $R_5^- \cup h$. Clearly, $H[R_5^- \cup h]$ has seven 2-degree vertices. If $r \geq 3$, then the territory $T[R_5^- \cup h]$ of $R_5^- \cup h$ has at most four 2-degree vertices on its boundary. By Lemma 2.2, $n \leq |V(T[R_5^- \cup h])| + 2 \leq 26 + 2 = 28$, contradicting that $n \geq 40$. So suppose $r \leq 2$.

If $r = 2$, then the boundary of $T[R_5^- \cup h]$ has five 2-degree vertices which separate $\partial(T[R_5^- \cup h])$ into five degree-saturated paths. If $f_2$ is a pentagon, $\partial(T[R_5^- \cup h])$ has four 2-length degree-saturated paths and one 3-length degree-saturated path (see Fig. 6(b)). Then the hexagon extension $H[T[R_5^- \cup h]]$ has only four 2-degree vertices on its boundary. By Lemma 2.2 and Proposition 2.4, $n \leq |V(H[T[R_5^- \cup h]])| + 2 = |V(T[R_5^- \cup h])| + 9 + 2 = 38$, contradicting $n \geq 40$. So suppose $f_2$ is a hexagon. If the two pentagons in $\{f_1, f_3, f_4, f_5, f_6\}$ are adjacent, $\partial(T[R_5^- \cup h])$ has one 1-length degree-saturated path and three 2-length degree-saturated paths and one 4-length degree-saturated path (see Fig. 6(c)). Then $H[T[R_5^- \cup h]]$ has 35 vertices and three 2-degree vertices. By Lemma 2.2 and Proposition 2.4, $n \leq |V(H[T[R_5^- \cup h]])| + 1 = 36$, contradicting that $n \geq 40$. So we suppose the two pentagons in $\{f_1, f_3, f_4, f_5, f_6\}$ are not adjacent. Then $\partial(T[R_5^- \cup h])$ has one 1-length degree-saturated path and two 2-length degree-saturated paths and two 3-length degree-saturated paths (see Fig. 6(d)). Further, $H[T[R_5^- \cup h]]$ has 36 vertices and four 2-degree vertices. By Lemma 2.2 and Proposition 2.4, $n \leq |V(H[T[R_5^- \cup h]])| + 2 = 38$, also contradicting that $n \geq 40$.

So $r = 1$. Suppose $h \in \mathcal{H}$. Then $f_1, f_2, f_3 \notin \mathcal{H}$. If $f_4, f_6 \in \mathcal{H}$, then $R_5^- \cup h - \mathcal{H}$ has no matchings which cover all remaining 3-degree vertices of $R_5^- \cup h$, a contradiction. So at most one of $\{f_4, f_5, f_6\}$ belongs to $\mathcal{H}$. Hence, $|U_{\mathcal{H}}(R_5^-)| = |V(R_5^- \cup h)| - |V(\mathcal{H})| \geq 16 - 9 = 7$. Since $G$ has $k$ pentagons and $r = 1$, it holds that $G - R_5^-$ has at least $k - 6$ pentagons. By Lemma 2.7, $|U_{\mathcal{H}}(G - R_5^-)| \geq k - 6$. Hence $|U_{\mathcal{H}}(G)| = |U_{\mathcal{H}}(R_5^-)| + |U_{\mathcal{H}}(G - R_5^-)| \geq 7 + k - 6 = k + 1$. Hence $G$ is not extremal.

Now suppose that $h \notin \mathcal{H}$. Since both $(R_5^- \cup h) - (\cup_{i=1,3,5} f_i)$ and $(R_5^- \cup h) - (\cup_{i=2,4,6} f_i)$ have no perfect matchings, at most two faces of $f_1, \ldots, f_6$ belong to $\mathcal{H}$. So $|U_{\mathcal{H}}(R_5^-)| \geq 14 - 6 = 8$. On the other hand, $G - R_5^-$ has $k - 6$ pentagons since $r = 1$. Hence, by Lemma 2.7, $|U_{\mathcal{H}}(G)| = |U_{\mathcal{H}}(R_5^-)| + |U_{\mathcal{H}}(G - R_5^-)| \geq 8 + k - 6 \geq k + 2$, a contradiction. Hence $G$ is not extremal. □

For a pentagonal fragment $B$, let $\gamma(B)$ be the minimum number of pentagons adjoining a common pentagon in $B$. Let $B^*$ be the inner dual of $B$. Then $\gamma(B)$ is the the minimum degree of $B^*$. For example, $\gamma(R_5) = 3$ and $\gamma(R_5^-) = 2$.

**Lemma 3.6.** *Let $B$ be a pentagonal fragment of a fullerene graph $F$. Then:*

(1) *$R_5 \subseteq B$ if $\gamma(B) \geq 3$;*
(2) *$B$ has a pentagon adjoining exactly two adjacent pentagons of $B$ if $\gamma(B) = 2$.*

**Proof.** Let $B^*$ be the inner dual of $B$. Then $B^*$ is a simple connected graph and every inner face of $B^*$ is a triangle. Let $\delta(B^*)$ be the minimum degree of $B^*$. Then $\delta(B^*) = \gamma(B)$.

Suppose to the contrary that $R_5 \not\subseteq F$; that is, $B^*$ is an outer plane graph. It suffices to prove that $\delta(B^*) \leq 2$ and $B^*$ has a 2-degree vertex on a triangle of $B^*$ if $\delta(B^*) = 2$. If $\delta(B^*) = 1$, the assertion already holds. So suppose $\delta(B^*) = 2$. Let $G$ be a maximal 2-connected subgraph of $B^*$ such that $G$ is connected to $F - G$ by an edge $e$. If $B^*$ is 2-connected, let $G = B^*$. Then every inner face of $G$ is a triangle. So it suffices to prove that $G$ has two 2-degree vertices.

Let $C$ be the boundary of $G$. Let $v_0, v_1, v_2, \ldots, v_{n-1}$ be all vertices of $G$ appearing clockwise on $C$. If $n = 3$, then $G$ is a triangle and the assertion is true. So suppose $n > 3$. Since every inner face of $G$ is a triangle, then $G$ has 3-degree vertices. Without loss of generality, let $v_0$ be a 3-degree vertex such that $v_0v_k$ is a chordal of $C$ where $k \neq 1, n-1$. Let $v_jv_{j'}$ be a chordal of $C$ such that $k \leq j < j+1 < j' \leq n \equiv 0 \pmod n$ and $|j' - j|$ is minimal. Then the cycle $v_jv_{j+1} \cdots v_{j'-1}v_{j'}v_j$ bounds an inner face. So it is a triangle and $v_{j+1}$ is a 2-degree vertex on the triangle $v_jv_{j+1}v_{j'}v_j$. On the other hand, let $v_iv_{i'}$ be a chordal of $C$ such that $0 \leq i < i+1 < i' \leq k$ and $i' - i$ is minimal. A similar analysis implies that $v_{i+1}$ is a 2-degree vertex on the triangle $v_iv_{i+1}v_{i'}v_i$. At most one of $v_{j+1}$ and $v_{i+1}$ is an end of the edge $e$ joining $G$ to $F - G$. So $B$ has a 2-degree vertex on a triangle of $B$. This completes the proof of the lemma. □

**Lemma 3.7.** *Let $B$ be a pentagonal fragment with $\gamma(B) \geq 2$. Then $B$ is not extremal.*

**Proof.** Let $k$ be the number of pentagons of $B$ and $\mathcal{H}$ be a Clar set of $H[G]$. Use induction on $k$ to prove it. The minimum pentagonal fragment $B_0$ with $\gamma(B_0) \geq 2$ consists of three pentagons such that they adjoin each other. It is easy to verify that $B_0$ is not extremal. So we may suppose $k \geq 4$ and the lemma holds for smaller $k$. If $R_5 \subseteq B$, then $B$ is not extremal according to Observation 3.3. By Lemma 3.6, we may assume $\gamma(B) = 2$ and let $p := v_1v_2v_3v_4v_5v_1$ be a pentagon of $B$ adjoining two pentagons $p_1$ and $p_2$ such that $p_1 \cap p = v_3v_4$ and $p_2 \cap p = v_4v_5$.

Let $h_1, h_2, h_3$ be the three hexagons of $F_n$ adjoining $p$ as illustrated in Fig. 7(a). If one of $v_1$ and $v_2$ belongs to $U_{\mathcal{H}}(B)$, then $B' := B - \{v_1, v_2\}$ has at least $k - 1$ pentagons and $\gamma(B') \geq 2$. So $B' \notin \mathscr{B}_{\geq 60}$. By inductive hypothesis, $B'$ is not extremal and hence $|U_{\mathcal{H}}(B')| \geq k$. Hence $|U_{\mathcal{H}}(B)| \geq |V(B') \cap U_B| + 1 \geq k + 1$. That means $B$ is also not extremal. So suppose $v_1, v_2 \in V(\mathcal{H})$. Then either $h_2 \in \mathcal{H}$ or $h_1, h_3 \in \mathcal{H}$.

*Case* 1: $h_2 \in \mathcal{H}$. Then $v_3, v_4, v_5 \in U_{\mathcal{H}}(B)$ and all of them are covered by $M_B$. Let $f_1, f_2$ be the other two faces adjoining $p_1$ as shown in Fig. 7(a). Let $w_1v_4 = p_1 \cap p_2$. If $f_2 \notin \mathcal{H}$, then $S = \{w_1, v_3, v_4, v_5\} \subseteq U_{\mathcal{H}}(B)$, a contradiction. So suppose $f_2 \in \mathcal{H}$.

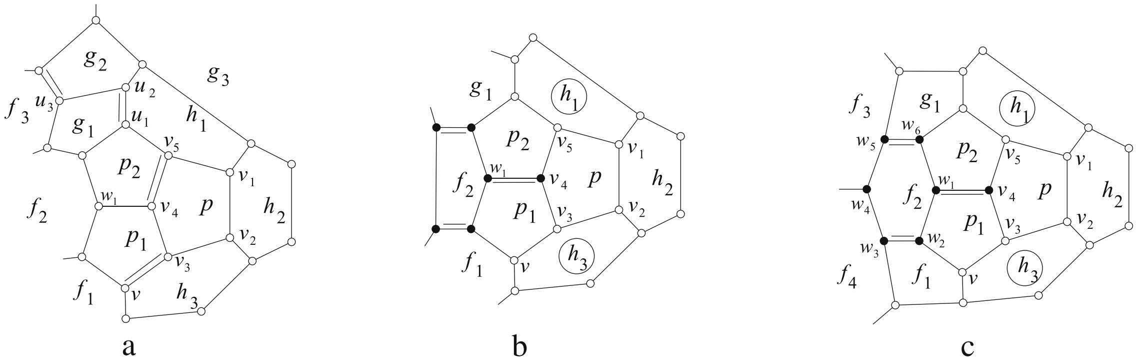


**Fig. 7.** Illustration for the proof of Lemma 3.7.

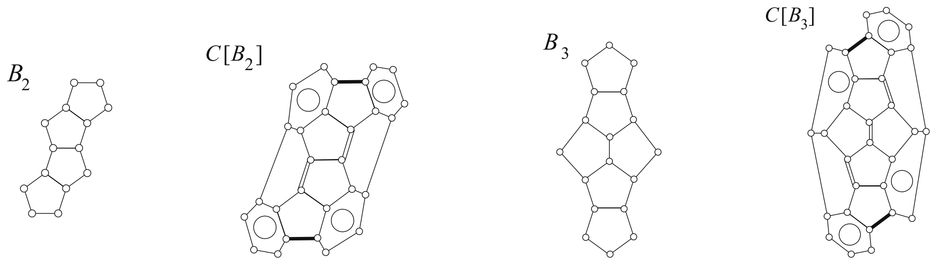


**Fig. 8.** Extremal pentagonal fragments $B_2$, $B_3$ and their Clar extensions $C[B_2]$, $C[B_3]$.

So either $v_3v_4 \in M_B$ or $v_4v_5 \in M_B$. By symmetry, we may assume $v_4v_5 \in M_B$. Let $vv_3 = p_1 \cap h_3$. Then $vv_3 \in M_B$. Since $\{v_3, v_4, v_5, v\} \subseteq U_{\mathcal{H}}(B)$ should meet at least four pentagons, $f_1$ is a pentagon.

Let $g_1, g_2, g_3$ be the faces adjoining $h_1$ as illustrated in Fig. 7(a), and let $u_1u_2 = g_1 \cap h_1$ and $u_2u_3 = g_1 \cap g_2$. Since $g_1 \notin \mathcal{H}$, we have $u_1 \in U_{\mathcal{H}}(B)$. Since $\{v_3, v_4, v_5, u_1\} \subseteq U_{\mathcal{H}}(B)$ meets at least four pentagons, $g_1$ is a pentagon. Hence $u_1u_2 \in M_B$. So $\{v_3, v_4, v_5, u_1, u_2\} \subseteq U_{\mathcal{H}}(B)$. Further $g_2$ is also a pentagon. Let $f_3$ be the face adjoining $g_1, g_2$ and $f_2$. Then $f_3 \notin \mathcal{H}$ since it is adjacent with $f_2$. Further, $f_3$ is a pentagon since $\{v_3, v_4, v_5, u_1, u_2, u_3\} \subseteq U_{\mathcal{H}}(B)$ meets at least six pentagons.

Let $B' := B - (V(P) \cup \{w_1\})$. If $B'$ is connected, then the pentagons in $B'$ connecting $f_1$ and $g_1$ together with $p_1, p_2$ form a pentagonal ring in $B$, contradicting that $B$ is a pentagonal fragment. Let $B_1, \ldots, B_r$ be all components of $B'$ such that $g_1 \subseteq B_1$. Use $k_i$ to denote the number of pentagons in $B_i$, then $k = \sum_{i=1}^{r} k_i + 3$. For $B_1$, we have $\gamma(B_1) \geq 2$ and hence $B_1 \notin \mathscr{B}_{\geq 60}$. By inductive hypothesis, $B_1$ is not extremal. So $|U_{\mathcal{H}}(B_1)| \geq k_1 + 1$. By Lemma 2.7, $|U_{\mathcal{H}}(B)| = \sum_{i=1}^{r} |U_{\mathcal{H}}(B_i)| + 3 \geq (k_1 + 1) + \sum_{i=2}^{r} k_i + 3 = k + 1$. So $B$ is not extremal.

*Case* 2: $h_1, h_3 \in \mathcal{H}$. Let $w_1v_3 = p_1 \cap p_2$. Then $w_1v_3 \in M_B$. Let $f_1, f_2, g_1$ be the other three faces adjoining $p_1$ or $p_2$ (see Fig. 7(b)). If $f_2$ is a pentagon, then $V(f_2) \subseteq U_{\mathcal{H}}(B)$ since $f_1, g_1 \notin \mathcal{H}$. Hence $V(f_2)$ meets at least five pentagons. That means $f_2$ is adjacent with at least four pentagons in $B$, forming a $R_5^-$ in $B$. So $B$ is not extremal by Lemma 3.5. So suppose $f_2$ is a hexagon. Clearly, $f_2 \notin \mathcal{H}$ since $w_1 \in U_{\mathcal{H}}(B)$.

Since $\gamma(B) = 2$, both $g_1$ and $f_1$ are pentagons. Let $f_2 := w_1w_2w_3w_4w_5w_6w_1$ and let $f_3, f_4$ be the other two faces adjoining $f_2$ (see Fig. 7(c)). Since $B$ is a pentagonal fragment, at most one of $f_3$ and $f_4$ is a pentagon. If exactly one of them is a pentagon, then $V(f_2) \subseteq U_{\mathcal{H}}(B)$ meets only five pentagons, a contradiction. So suppose both of them are hexagons. Then $\{w_1, w_2, w_3, w_5, w_6\} \subseteq U_{\mathcal{H}}(B)$ meets only four pentagons, also a contradiction. So $B$ is not extremal. $\square$

Now, we are going to characterize extremal pentagonal fragments. Let $B_2, B_3$ be the two pentagonal fragments illustrated in Fig. 8. Clearly, the Clar extensions of $B_2$ and $B_3$ are normal. It is easy to see that $P, B_2$ and $B_3$ are extremal. Up to isomorphism, $C[P]$, $C[B_2]$ and $C[B_3]$ are unique.

Let $G_1, G_2, G_3$ and $G_4$ be graphs. We say that $G_1$ arises from *pasting* $G_2$ and $G_3$ along $G_4$ if $G_1 = G_2 \cup G_3$ and $G_4 = G_2 \cap G_3$. Let $B$ be a fragment isomorphic to one of $P, B_2$ and $B_3$ and let $C[B]$ be a Clar extension of $B$. An edge of $B$ is called *pasting edge* if it lies on the boundary of $C[B]$ and two end-vertices belong to $V(\mathcal{H})$ where $\mathcal{H}$ is the Clar set of $C[B]$. The thick edges of $P, B_2$ and $B_3$ illustrated in Figs. 8 and 9 are pasting edges. We can paste $P, B_2, B_3$ with each other or itself along the pasting edges to form a new pentagonal fragment. Use "$*$" to denote the pasting operation. Up to isomorphism, $P * P$ and $P * B_2$ are illustrated in Fig. 9. Simply, use $X^k$ to denote the graph obtained pasting $k$ graphs isomorphic to $X$ along the pasting edges together, where $X \in \{P, B_2, B_3\}$. Note that the pasting operation does not always yield a subgraph of a fullerene graph. Let $\mathscr{B}$ be the set of all maximal pentagonal fragments, which are subgraphs of some fullerene graph, generated from the pasting operation. Let $\mathscr{B}_{\geq 60} \subset \mathscr{B}$ such that $B \subset F_n$ $(n \geq 60)$ for any $B \in \mathscr{B}_{\geq 60}$.

**Lemma 3.8.** $B_2 * B_3, B_3^2 \notin \mathscr{B}$.

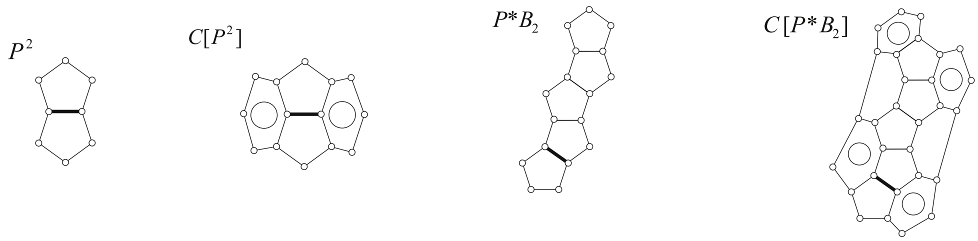


**Fig. 9.** The pasting operation: $P^2, P * B_2$ and their Clar extensions.

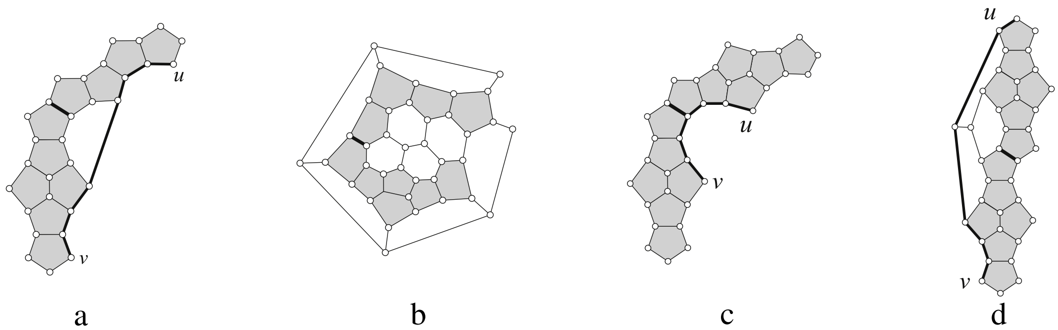


**Fig. 10.** $B_2 * B_3$ (grey graphs in (a) and (b)) and $B_3^2$ (grey graphs in (c) and (d)).

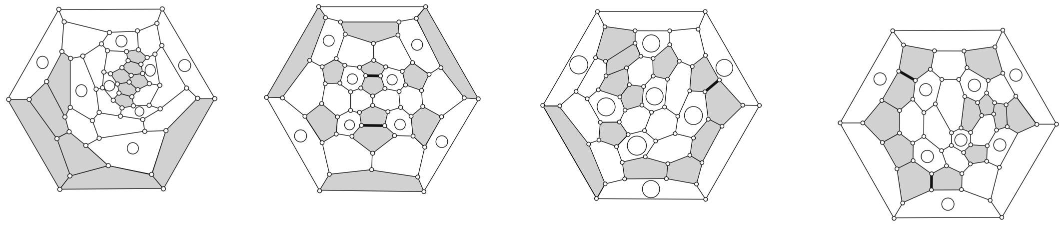

**Fig. 11.** Extremal fullerene graphs with 60 vertices.

**Proof.** Up to isomorphism, all cases of $B_2 * B_3$ and $B_3^2$ are illustrated as the graphs in grey color in Fig. 10. Suppose to the contrary that $B_2 * B_3$, $B_3^2 \in \mathscr{B}$. Then the hexagon extension of $B_2 * B_3$, $B_3^2$ are subgraphs of fullerene graphs. So all graphs illustrated in Fig. 10 are fragments of fullerene graphs, contradicting either Proposition 2.3 or Lemma 2.2. So $B_2 * B_3, B_3^2 \notin \mathscr{B}$. □

We are particularly interested in the graphs in $\mathscr{B}_{60}$. From the extremal fullerene graphs shown in Fig. 11, we can easily see that $\{P, B_2, B_3, P^2, P * B_2, P * B_2 * P\} \subseteq \mathscr{B}_{\geq 60}$. In fact, these two sets are equal.

**Lemma 3.9.** $\mathscr{B}_{\geq 60} = \{P, B_2, B_3, P^2, P * B_2, P * B_2 * P\}$.

**Proof.** It is clear that $\{P, B_2, B_3, P^2, P * B_2, P * B_2 * P\} \subseteq \mathscr{B}_{\geq 60}$. In the following, we will prove another direction that $\mathscr{B}_{\geq 60} \subseteq \{P, B_2, B_3, P^2, P * B_2, P * B_2 * P\}$. By Lemma 3.8, it suffices to prove $B_2^2 \nsubseteq B$ and $B_3 * P \nsubseteq B$ for any $B \in \mathscr{B}_{\geq 60}$.

Suppose $B_2^2 \subseteq B \in \mathscr{B}_{\geq 60}$. Clearly, $B_2^2$ has two cases as shown in Fig. 12 (the grey subgraphs in (a) and (c)). Their Clar extensions $C[B_2^2] \subseteq H[B] \subseteq F_n$ are graphs (a) and (c) in Fig. 12. The corresponding hexagon extensions $H[C[B_2^2]]$ are graphs (b) and (d) in Fig. 12. Since $H[C[B_2^2]]$ has four 2-degree vertices, $n \leq V(T[C[B_2^2]]) + 2 \leq V(H[C[B_2^2]]) + 2 \leq 56$ by Lemma 2.2 and Proposition 2.4, contradicting that $n \geq 60$. Hence, $B \notin \mathscr{B}_{\geq 60}$.

Now suppose $B_3 * P \subseteq B \in \mathscr{B}_{\geq 60}$. Its Clar extension $C[B_3 * P] \subset H[B] \subseteq F_n$ and $H[C[B_3 * P]]$ are illustrated in Fig. 13. Let $f$ be the face adjoining $H[C[B_3 * P]]$ as shown in Fig. 13. Let $G := H[C[B_3 * P]] \cup f$. Then $G$ has at most four 2-degree vertices. So $n \leq |V(G)| + 2 \leq V(H[C[B_3 * P]]) + 3 = 44$ by Lemma 2.2 and Proposition 2.4, contradicting that $n \geq 60$. So $B \notin \mathscr{B}_{\geq 60}$. □

**Theorem 3.10.** *Let $B$ be a maximal pentagonal fragment of fullerene graph $F_n$ ($n \geq 60$). Then $B$ is extremal if and only if $B \in \mathscr{B}_{\geq 60}$.*

**Proof.** By Lemma 3.9 and the extremal fullerene graphs in Fig. 11, the sufficiency is obvious. So it suffices to prove the necessity. Let $B$ be a maximal extremal pentagonal fragment with $k$ pentagons in $F_n$ ($n \geq 60$). We use induction on $k$ to prove $B \in \mathscr{B}_{\geq 60}$. Let $\mathscr{H}$ be a Clar set of $H[B]$ and $M_B$ be the matching of $B - \mathscr{H}$ which covers all remaining 3-degree vertices

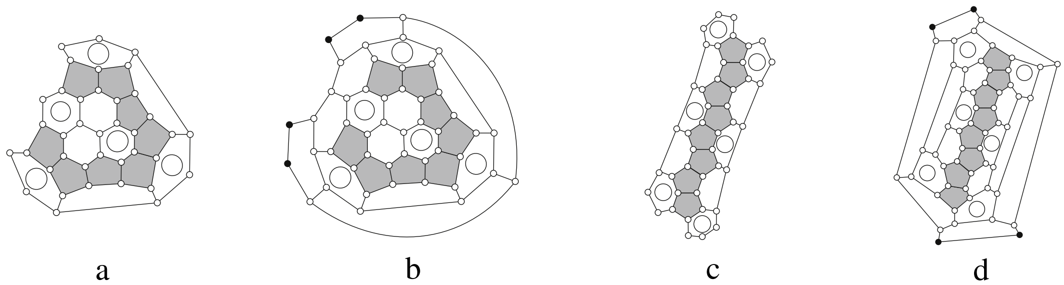


**Fig. 12.** Clar extensions $C[B_2^2]$ ((a) and (c)) and their hexagon extensions ((b) and (d)).

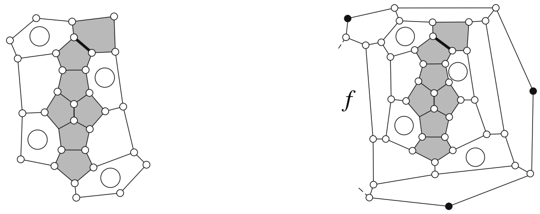


**Fig. 13.** Graphs $C[B_3 * P]$ (left) and $H[C[B_3 * P]]$ (right).

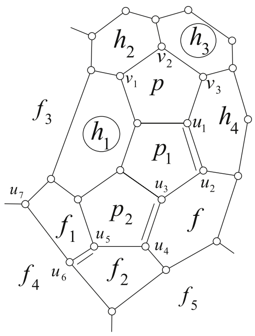


**Fig. 14.** Pentagonal fragment $B$ with $h_1, h_3 \in \mathcal{H}$.

of $B$. Let $S$ be a subset of $V(B)$ meeting at most $|S| - 1$ pentagons in $B$. If $S \subseteq U_{\mathcal{H}}(B)$, then $B - S$ has $k + 1 - |S|$ pentagons and then has at least $k + 1 - |S|$ vertices in $U_{\mathcal{H}}(B)$ by Lemma 2.7. Hence $|U_{\mathcal{H}}(B)| \geq k + 1$, contradicting that $B$ is extremal. So, in the following, we may assume that $U_{\mathcal{H}}(B)$ contains no such $S$.

For $k = 1$ or 2, then $B = P$ or $P^2$. The necessity holds since $P, P^2 \in \mathscr{B}_{\geq 60}$. Now suppose that $k \geq 3$ and the necessity holds for smaller $k$. Let $p, p_1, p_2$ be the three pentagons of $B$. By Lemma 3.7, $\gamma(B) = 1$. Let $p$ be the pentagon adjoining only one pentagon, say $p_1$, along an edge $e$ and $V(p) - V(e) = \{v_1 v_2, v_3\}$. Enumerate clockwise the hexagons in $F_n$ adjoining $p$ as $h_1, h_2, h_3$ and $h_4$ (see Fig. 14). Since any two vertices in $\{v_1, v_2, v_3\}$ form a vertex set $S$, it follows that $U_{\mathcal{H}}(B)$ contains at most one of $v_1$, $v_2$ and $v_3$.

If one of $v_1$ and $v_3$ belongs to $U_{\mathcal{H}}(B)$, say $v_1$, then $h_3 \in \mathcal{H}$ since $v_2, v_3 \in V(\mathcal{H})$. So $h_1, h_4 \notin \mathcal{H}$. Let $S := \{v_1\} \cup V(p \cap p_1)$. Then $S \subseteq U_{\mathcal{H}}(B)$, contradicting the assumption. If $v_2 \in U_B$, then $h_1, h_2 \in \mathcal{H}$. Let $B' := B - \{v_1, v_2, v_3\}$. Then $B'$ has $k - 1$ pentagons and $|U_{\mathcal{H}}(B')| = k - 1$. By the inductive hypothesis, $B' \in \mathscr{B}_{\geq 60}$. So $B$ arises from pasting $B'$ and $p$ along $p \cap p_1$ and hence $B \in \mathscr{B}_{\geq 60}$ by Lemma 3.9. From now on, suppose $v_1, v_2, v_3 \in V(\mathcal{H})$.

First suppose $h_1, h_3 \in \mathcal{H}$. Let $u_1 u_2 = p_1 \cap h_4$. Then $u_1 u_2 \in M_B$. If $f$ is a pentagon, by the symmetry and a similar discussion as that of Subcase 1.1, we have $B = B_3 \in \mathscr{B}_{\geq 60}$. So suppose $f$ is a hexagon. Then $f \notin \mathcal{H}$ since $u_2 \in V(f) \cap V(\mathcal{H})$. Let $u_3 u_4 = p_2 \cap f$. Then $u_3 u_4 \in M_B$. Let $f_1, f_2$ be other two faces adjoining $p_2$ as illustrated in Fig. 14. Since $\{u_1, \ldots, u_4\} \subseteq U_{\mathcal{H}}(B)$ meets at least four pentagons, $f_2$ is a pentagon. Let $u_5 u_6 = f_1 \cap f_2$. Then $u_5 u_6 \in M_B$ since $f_1 \notin \mathcal{H}$. Let $f_3, f_4, f_5$ be the other three faces adjoining $f_1$ or $f_2$. Since $\{u_1, \ldots, u_6\} \subseteq U_{\mathcal{H}}(B)$ should meet at least six pentagons, both $f_1$ and $f_4$ are pentagons. Let $u_6 u_7 = f_1 \cap f_4$. Then $u_7 \in U_{\mathcal{H}}(B)$ because $f_3 \notin \mathcal{H}$. Since $\{u_1, \ldots, u_7\} \subseteq U_{\mathcal{H}}(B)$ meets at least seven pentagons, $f_3$ is also a pentagon. So $R_5^- = f_1 \cup f_2 \cup f_3 \cup f_4 \cup p_2 \subseteq B$. By Lemma 3.5, $B$ is not extremal.

So, in the following, suppose $h_2, h_4 \in \mathcal{H}$. Let $f$ be the face adjoining $p_1$, $p_2$ and $h_4$, and let $u_1 u_2 = h_1 \cap p_1$ and $u_3 u_4 = f \cap p_2$ (see Fig. 15(a)). Then $u_1 u_2, u_3 u_4 \in M_B$.

First suppose $f$ is a hexagon. Let $f_1$ and $f_2$ be the other two faces adjoining $p_2$, distinct from $h_1$, $p_1$ and $f$ (see Fig. 15(a)). Since $\{u_1, u_2, u_3, u_4\}$ meets at least 4 pentagons, $f_2$ is a pentagon. If $f_1 \notin \mathcal{H}$, then $S = V(p_2) \subseteq U_{\mathcal{H}}(B)$, contradicting

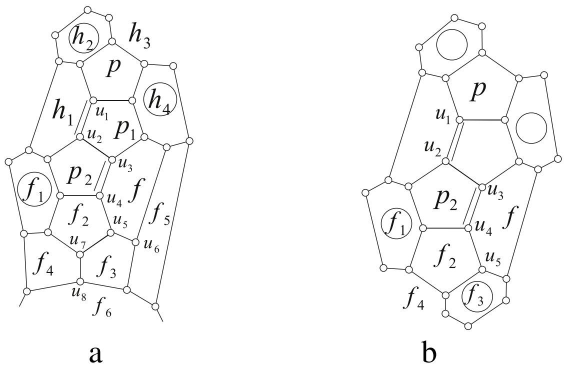


**Fig. 15.** Illustration for the proof of Theorem 3.10.

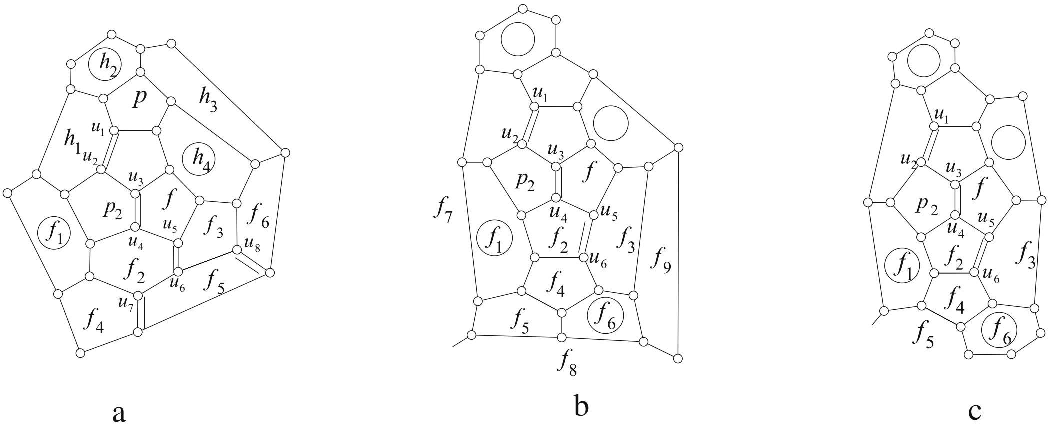


**Fig. 16.** Illustration for the proof of Theorem 3.10.

the assumption. So $f_1 \in \mathcal{H}$. Let $u_4u_5 = f_2 \cap f$ and let $f_3, f_4 \neq p_2$ be the other two faces adjoining both $f_2$ as shown in Fig. 15(a). If $f_3 \notin \mathcal{H}$, then $f_3$ is a pentagon since $\{u_1, \dots, u_5\} \subseteq U_{\mathcal{H}}(B)$ meets at least five pentagons. Let $u_5u_6 = f \cap f_3$ and $u_7u_8 = f_3 \cap f_4$. Clearly, $u_6, u_7 \in U_{\mathcal{H}}(B)$. Let $f_5, f_6$ be two faces adjoining $f_3$ as shown in Fig. 15(a). Since both $\{u_1, u_2, \dots, u_5, u_6\}$ and $\{u_1, u_2, \dots, u_5, u_7\}$ meet at least six pentagons, both $f_5$ and $f_4$ are pentagonal. If $f_6$ is a pentagon, then $f_2, f_3, f_4, f_5$ and $f_6$ form a $R_5^- \subseteq B$, contradicting Lemma 3.5. So $f_6$ is a hexagon. Clearly, $f_6 \notin \mathcal{H}$ because $\{u_5u_6, u_7u_8\} \subset M_B$ or $\{u_5u_7, f_3 \cap f_5\} \subset M_B$. So $S := V(f_3) \subseteq U_{\mathcal{H}}(B)$, a contradiction. The contradiction implies that $f_3 \in \mathcal{H}$. Hence $p \cup p_1 \cup p_2 \cup f_2 = B_2$ and $f_2 \cap f_4$ is a pasting edge (see Fig. 15(b)). If $f_4$ is a hexagon, then $B = B_2 \in \mathscr{B}_{\geq 60}$. If $f_4$ is a pentagon, let $B' := B - (p_1 \cup p_2 \cup p \cup \{u_5\})$. Then $B'$ has $k - 4$ pentagons and $|U_{\mathcal{H}}(B')| = k - 4$. By inductive hypothesis, $B' \in \mathscr{B}_{\geq 60}$. Hence, $B$ arises from pasting $B'$ and $B_2$ along $f_2 \cap f_4$. Therefore, $B \in \mathscr{B}_{\geq 60}$ by Lemma 3.9.

Now suppose that $f$ is a pentagon (see Fig. 16). Let $u_5u_6 = f_2 \cap f_3$. Then $f_1$ (or $f_3$) and $f_2$ cannot be pentagonal simultaneously by Lemma 3.8. Since $u_3u_4 \in M_B$, we have $f_2 \notin \mathcal{H}$. Clearly $f_3 \notin \mathcal{H}$. So $\{u_1, \dots, u_5\} \subseteq U_{\mathcal{H}}(B)$. Hence $\{u_1, \dots, u_5\}$ meets at least five pentagons. So at least one of $f_2$ and $f_3$ is pentagonal.

If $f_3$ is a pentagon, then $f_2$ is a hexagon and $u_5u_6 \in M_B$ by Lemma 3.5. Let $f_4, f_5$ and $f_6$ be the other three faces adjoining $f_2$ or $f_3$ as illustrated in Fig. 16(a). Let $u_6u_7 = f_2 \cap f_5$ and $u_6u_8 = f_3 \cap f_5$. Since both $\{u_1, \dots, u_6, u_7\} \subseteq U_{\mathcal{H}}(B)$ and $\{u_1, \dots, u_6, u_8\} \subseteq U_{\mathcal{H}}(B)$ meet at least seven pentagons, all $f_4, f_5, f_6$ are pentagonal. Hence $f_4 \cap f_5 \in M_B$ and $f_5 \cap f_6 \in M_B$. So $S := V(f_5) \subseteq U_{\mathcal{H}}(B)$ meets only four pentagons in $B$, a contradiction.

So suppose that $f_2$ is a pentagon and both $f_1$ and $f_3$ are hexagons (see Fig. 16(b)). Clearly, $f_3 \notin \mathcal{H}$ and $u_5u_6 \in M_B$ since $h_4 \in \mathcal{H}$. Since $V(f_2)$ meets four pentagons, $V(f_2) \nsubseteq U_{\mathcal{H}}(B)$ and hence $f_1 \in \mathcal{H}$. Let $f_4$ be the face adjoining $f_1, f_2$ and $f_3$. Then $f_4$ is a pentagon since $\{u_1, \dots, u_6\}$ meets at least six pentagons. Let $f_5$ and $f_6$ be the faces adjoining $f_4$ as illustrated in Fig. 16(b). Clearly, $f_5 \notin \mathcal{H}$ since it is adjacent with $f_1 \in \mathcal{H}$.

If $f_6 \notin \mathcal{H}$, then $V(f_4 \cap f_6) \subset U_{\mathcal{H}}(B)$. Both $f_5$ and $f_6$ are pentagons since $\{u_1, \dots, u_6\} \cup V(f_4 \cap f_6) \subseteq U_{\mathcal{H}}(B)$ meets at least 8 pentagons. Let $f_7, f_8$ and $f_9$ be faces adjoining $f_5$ or $f_6$ as illustrated in Fig. 16(b). Since $\{u_1, \dots, u_6\} \cup V(f_3 \cap f_6) \subseteq U_{\mathcal{H}}(B)$, we have $f_9$ is a pentagon of $B$. Since $\{f_3 \cap f_6, f_5 \cap f_6\} \subset M_B$ or $\{f_4 \cap f_6, f_6 \cap f_9\} \subset M_B$, we have $f_8 \notin \mathcal{H}$. Further, $f_8$ is a hexagon because $R_5^- \nsubseteq B$. Hence $S := V(f_6) \subseteq U_{\mathcal{H}}(B)$ meets only four pentagons in $B$, a contradiction.

So suppose that $f_6 \in \mathcal{H}$. Then $p \cup p_1 \cup p_2 \cup f \cup f_2 \cup f_4 = B_3$ (see Fig. 16(c)). By the proof of Lemma 3.8, we have $B = B_3 \in \mathscr{B}_{\geq 60}$. This completes the proof of the theorem. $\square$

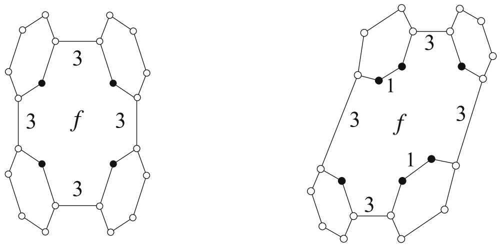


**Fig. 17.** The boundary labelings: 3333 (right) and 331331 (left).

Let $F_n$ ($n \geq 60$) be an extremal fullerene graph. That means $c(F_n) = \frac{n-12}{6}$. By Lemma 3.1 and Theorem 3.10, every pentagon of $F_n$ lies in a pentagonal fragment $B \in \mathscr{B}_{\geq 60}$. For a Clar formula $\mathscr{H}$ of $F_n$ and a maximal pentagonal fragment $B$ of $F_n$, we have that $\mathscr{H} \cap H[B]$ is a Clar set of $H[B]$ where $H[B]$ is the hexagon extension of $B$.

**Theorem 3.11.** *Let $F_n$ ($n \geq 60$) be a fullerene graph and $B_1, B_2, \ldots, B_k$ be all maximal pentagonal fragments of $F_n$. Then $F_n$ is extremal if and only if*

(1) *$B_i \in \mathscr{B}_{\geq 60}$ for all $1 \leq i \leq k$; and*
(2) *$H[\cup_{i=1}^{k} B_i]$ has a normal Clar set $\cup_{i=1}^{k} \mathscr{H}_i$ where $\mathscr{H}_i$ is the Clar set of $H[B_i]$; and*
(3) *$F_n - C[\cup_{i=1}^{k} B_i]$ has a sextet pattern covering all vertices in $V(F_n - C[\cup_{i=1}^{k} B_i])$.*

Theorem 3.11 gives a characterization of extremal fullerne graphs. This characterization provides an approach to construct all extremal fullerene graphs with 60 vertices.

## 4. Extremal Fullerene graphs with 60 vertices

Let $F_n$ be an extremal fullerene graph and $\mathscr{H}$ be a Clar formula of $F_n$. Then $|\mathscr{H}| = \frac{n-12}{6}$ and $M := F_n - \mathscr{H}$ is a matching with six edges. By Theorem 3.11, every pentagon lies in a maximal extremal pentagonal fragment $B \in \mathscr{B}_{\geq 60}$ and $\mathscr{H} \cap H[B]$ is a Clar set of $H[B]$ where $H[B]$ is the hexagon extension of $B$. Then $M_B = E(B) \cap M$ is the matching of $B$ covering all 3-degree vertices of $B$ in $V(B - \mathscr{H})$. For $B = P^2$, or $B_2 * P$ or $P * B_2 * P$, every $P$ has a vertex $v$ uncovered by $M_B$. Obviously, $v$ is covered by $M$ and let $uv \in M$. Then $u$ belongs to another $P$. The edge $uv$ connects two $P$s to form a graph $B_1$ as illustrated in Fig. 3.

**Proposition 4.1.** *Let $\mathscr{H}$ be a Clar formula of an extremal fullerene graph $F_n$ ($n \geq 60$) and $M := F_n - \mathscr{H}$. Then a face $f$ of $F_n$ is a pentagon if and only if there exists an edge $e \in M$ such that $e \cap f \neq \emptyset$ and $e \notin E(f)$.* □

Let $G$ be a 2-connected subgraph of $F_n$. Then every face of $G$ is bounded by a cycle. Let $f$ be a face of $G$ with $k$ 2-degree vertices of $G$. Then $k$ 2-degree vertices separate $f$ into $k$ degree-saturated paths. Use a $k$-length sequence to label $f$ such that every numbers in the sequence correspond clockwise the lengths of all degree-saturated paths. The maximum one in the lexicographic order over all such $k$-length sequences is called the *boundary labeling* of $f$ (see Fig. 17).

**Proposition 4.2.** *Let $B$ be a fragment of an extremal fullerene graph $F_n$ and $\mathscr{H}$ be a Clar formula of $F_n$. Let $W$ be the set of all 2-degree vertices on $\partial B$. Then:*

(1) *$|W| \neq 1$;*
(2) *the boundary labeling of $\partial B$ is $ij$ with $5 \geq i \geq j \geq 4$ for $|W| = 2$;*
(3) *$|W| \neq 3$ for $W \subseteq V(\mathscr{H})$;*
(4) *the boundary labeling of $\partial B$ is 3333 or $i3j1$ with $5 \geq i \geq j \geq 4$ for $|W| = 4$ and $W \subseteq V(\mathscr{H})$.*

**Proof.** Since $B$ is a fragment, $\partial B$ is a cycle. Let $C := \partial B$. For convenience, we may draw $B$ on the plane such that $C$ bounds an inner face. All 2-degree vertices in $W$ separate $C$ into $|W|$ degree-saturated paths. Let $v \in W$ and $vv_1, vv_2 \in E(C)$. Let $v_3$ be the third neighbor of $v$ in $F_n$. Then $v_3$ lies in $F_n - B$ or $W$. Since $F_n$ is 3-connected, $|W| > 1$.

If $|W| = 2$, then the two 2-degree vertices are adjacent by Lemma 2.2. Since every face of $F_n$ is either a hexagon or a pentagon, the length of any degree-saturated path connecting the two 2-degree vertices is either 4 or 5. It follows that the boundary labeling of $\partial B$ is $ij$ with $5 \geq i \geq j \geq 4$.

If $|W| = 3$, then the 3-degree vertices have a common neighbor $u$ by Lemma 2.2. Since $W \subseteq V(\mathscr{H})$, it follows that $u$ is an isolate vertex of $F_n - \mathscr{H}$, contradicting that $\mathscr{H}$ is a Clar formula of $F_n$. So $|W| \neq 3$ if $W \subseteq V(\mathscr{H})$.

Now suppose $|W| = 4$. Let $u_0, u_1, u_2, u_3$ be the four vertices clockwise on $C$ (see Fig. 18). Let $P_{u_i,u_{i+1}}$ ($i, i+1 \in \mathbb{Z}_4$) be the degree-saturated path of $C$ connecting $u_i$ and $u_{i+1}$. Let $T := F_n - (V(B) \setminus W)$, the subgraph induced by the vertices within $C$ and the vertices in $W$. By Lemma 2.2, $T$ is $T_0$ or the union of two $K_2$s or a 3-length path. If $T$ is $T_0$, then the two vertices in the interior of $C$ are adjacent and hence induce an edge $e$. Then $e \in M := F_n - \mathscr{H}$. Let $f_1, f_2, f_3, f_4$ be the four faces meeting the edge $e$ (see Fig. 18(left)). By Proposition 4.1, both $f_1$ and $f_3$ are pentagonal. So $|P_{u_3,u_0}| = 4$ and $|P_{u_1,u_2}| = 4$. Since $5 \leq |f_3| \leq 6$ and $5 \leq |f_4| \leq 6$, we have that $u_0u_1 \notin E(F_n)$ and $u_2u_3 \notin E(F_n)$. Then $u_0$ and $u_1$ cannot be in the common hexagon in $\mathscr{H}$.

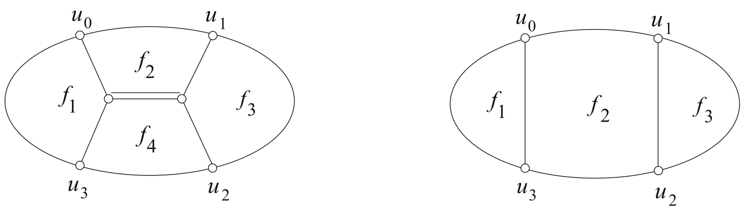


**Fig. 18.** Illustration for the proof of Proposition 4.2.

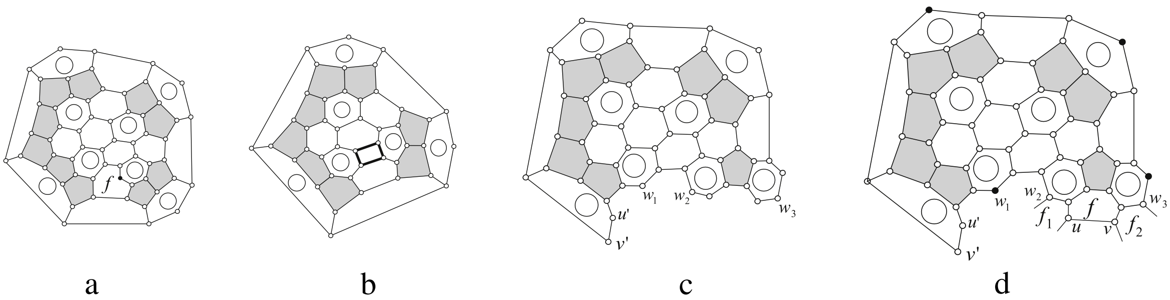


**Fig. 19.** Illustration for the proof of Lemma 4.3.

Similarly, $u_2$ and $u_3$ cannot be in the common hexagon in $\mathcal{H}$. So $|P_{u_0u_1}| = 4$ and $|P_{u_2u_3}| = 4$. Hence all $P_{u_i,u_{i+1}}$ for $i, i+1 \in \mathbb{Z}_4$ are 3-length path. Further, the boundary labeling of $\partial B$ is 3333.

If $G$ is the union of two $K_2$s or a 3-length path, then $u_0u_3, u_1u_2 \in E(F_n)$. Let $f_1, f_2, f_3$ be the three faces of $F_n$ within $C$ (see Fig. 18(right)). Hence $5 \leq |P_{u_0u_1}| \leq 6$ and $5 \leq |P_{u_2,u_3}| \leq 6$ since $5 \leq |f_1| \leq 6$ and $5 \leq |f_3| \leq 6$. Since $5 \leq |f_2| \leq 6$ and $\{u_0, u_1, u_2, u_3\} \subseteq V(\mathcal{H})$, then one of $|P_{u_0,u_1}|$ and $|P_{u_2,u_3}|$ equals 2 and the other equals 4. It follows that the boundary labeling of $\partial B$ is $i3j1$ with $5 \geq i \geq j \geq 4$. □

In the following, $F_{60}$ always means an extremal fullerene graph with 60 vertices. Using $B_1$ instead of $P$ in the pasting operation, let $\mathcal{G}_{60}$ denote the set of all maximal subgraphs of $F_{60}$ arising from the pasting operation on $B_1$, $B_2$ and $B_3$. Up to isomorphism, the Clar extension of $G \in \mathcal{G}_{60}$ is unique since the Clar extension of any element in $\mathcal{B}_{\geq 60}$ is unique. Note that $B_1^k$ is the graph obtained by pasting $k$ graphs isomorphic to $B_1$ along the pasting edge of each $P$ in $B_1$.

**Lemma 4.3.** $\mathcal{G}_{60} \subseteq \{B_1, B_2, B_3, B_1^2, B_1^3, B_1^4, B_1 * B_2, B_1 * B_2 * B_1, B_1 * B_2 * B_1 * B_2, B_2 * B_1 * B_2\}$.

**Proof.** Since $c(F_{60}) = 8$, we have that $B_1^k$ and $(B_1 * B_2)^r$ satisfy $k \leq 4$ and $r \leq 2$ if they belong to $\mathcal{G}_{60}$.

By Lemma 3.9, it suffices to prove $B_1^2 * B_2 \nsubseteq G$ for any $G \in \mathcal{G}_{60}$. Suppose to the contrary that $B_1^2 * B_2 \subseteq G \in \mathcal{G}_{60}$. Then either $G = B_1^3 * B_2$ or $G = B_1^2 * B_2$ by $c(F_{60}) = 8$.

If $G = B_1^3 * B_2$, then $B_1^3 * B_2$ has to be the grey subgraph of the graph (a) in Fig. 19 since $c(F_{60}) = 8$. The subgraph induced by $C[G]$ in $F_{60}$ is the graph (a) in Fig. 19. Proposition 4.2 implies that the graph (a) is not a subgraph of $F_{60}$. Hence $B_1^3 * B_2 \notin \mathcal{G}_{60}$, a contradiction.

If $G = B_1^2 * B_2$, then there are two cases for $G$ as the grey subgraphs illustrated in graphs (b) and (c) in Fig. 19, respectively. The graphs (b) and (c) are the subgraphs induced by $C[G]$. Clearly, the graph (b) could not be a subgraph of $F_n$ in that it has a 4-length cycle. For the graph (c), let $f$ be the hexagon adjoining $G$ along an edge of $B_1$ and $u, v, u', v', w_1, w_2, w_3$ be some 2-degree vertices on the boundary of $G \cup f$ (see Fig. 19(d)). If $uv \in E(\mathcal{H})$, then $u = u'$ and $v = v'$ since $F_{60}$ is a cubic plane graph. Then $w_1$ is adjacent to $w_2$ by Lemma 2.2, which forms a 4-length cycle in $F_{60}$, a contradiction. So suppose $uv \in M$. Let $f_1$ and $f_2$ be the pentagons met by $uv$ but not containing it by Proposition 4.1. Whether $uv \in M_{B_1}$ or $uv \in M_{B_2}$, one of $f_1$ and $f_2$ adjoins two hexagons in $\mathcal{H}$. So either $u'v' \in E(f_1)$ or $u'v' \in E(f_2)$. If $u'v' \in E(f_1)$, then $w_2$ is adjacent to $u'$ and hence $w_1$ would be a unique 2-degree on a face of a subgraph of $F_{60}$, contradicting Proposition 4.2. So suppose $u'v' \in E(f_2)$. Then $w_3$ is adjacent to $v'$, which forms a face with three 2-degree vertices which belong to $V(\mathcal{H} \cap C[G])$, also contradicting Proposition 4.2. So $B_1^2 * B_2 \notin \mathcal{G}_{60}$. This completes the proof. □

**Lemma 4.4.** *Let $G \subset F_{60}$ such that $G$ has two components, one of which is $B_1$ and another is $B_1$ or $B_2$. If the Clar extension $C[G]$ of $G$ is a fragment, then $|C[G] \cap \mathcal{H}| \geq 6$.*

**Proof.** Let $B_1$ and $B$ be two components of $G$, where $B$ is isomorphic to $B_1$ or $B_2$. By Theorem 3.11, the Clar set of $C[G]$ is a subset of a Clar formula $\mathcal{H}$ of $F_{60}$. Clearly, $|C[B_1] \cap \mathcal{H}| = 4$ and $|C[B] \cap \mathcal{H}| = 4$. Then $|C[G] \cap \mathcal{H}| = |(C[B_1] \cap \mathcal{H}) \cup (C[B] \cap \mathcal{H})| - |C[B_1] \cap C[B] \cap \mathcal{H}|$. If $|C[B_1] \cap C[B] \cap \mathcal{H}| \leq 2$, then $|C[G] \cap \mathcal{H}| \geq 6$ and the lemma is true.

So suppose $|C[B_1] \cap C[B] \cap \mathcal{H}| \geq 3$ and let $h_1, h_2, h_3 \in C[B_1] \cap C[B] \cap \mathcal{H}$ (see Fig. 20). Let $B' \subset C[B]$ be a fragment such that $B'$ contains $h_1, h_2, h_3$ and has minimal number of inner faces. Then $B'$ has at most 6 inner faces including $h_1$, $h_2$ and $h_3$

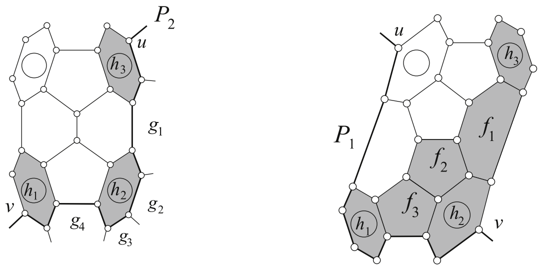


**Fig. 20.** Clar extensions of $B_1$ and $B_2$.

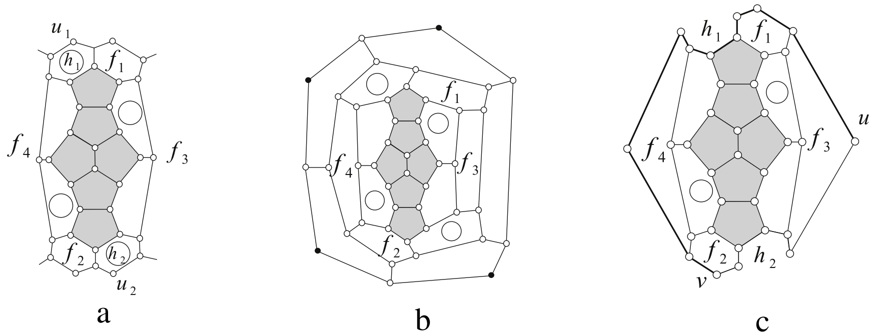


**Fig. 21.** Illustration for the proof of Lemma 4.5.

(see Fig. 20, the faces $f_1, f_2, f_3$ in $C[B_2]$) and $B' \cap C[B_1] = h_1 \cup h_2 \cup h_3$. Since $C[G]$ is a fragment, the faces of $B'$ different from $h_1, h_2, h_3$ adjoins $C[B_1]$. It needs at least 4 faces adjoining $C[B_1]$ to join $h_1$, $h_2$ and $h_3$ to form a fragment (the faces $g_1, \ldots, g_4$ in $C[B_1]$, see Fig. 20). So $B'$ has at least 7 inner faces, contradicting that $B'$ has at most 6 faces. The contradiction implies that $|C[B_1] \cap C[B] \cap \mathscr{H}| \leq 2$. So the lemma is true. □

**Lemma 4.5.** *If $B_3 \subset F_{60}$, then $F_{60}$ contains no other elements in $\mathscr{G}_{60}$ as subgraphs.*

**Proof.** Let $H[B_3]$ be the hexagon extension of $B_3$. Then $H[B_3] \subset F_{60}$. Let $f_1$ and $f_2$ be the two hexagons adjoining $B_3$ and let $f_3, f_4$ be two faces adjoining $C[B_3]$ as shown in Fig. 21(a).

Let $G_1 := H[B_3] \cup f_3 \cup f_4$. If at least one of $f_3$ and $f_4$, say $f_3$, is a pentagon. Then the hexagon extension $H[G_1]$ of $G_1$ contains at most four 2-degree vertices on its boundary (see Fig. 21(b)). By Lemma 2.2 and Proposition 2.4, it holds that $n \leq |V(G_1)| + 9 + 2 \leq 46$ if $G_1 \subset F_n$. So suppose both $f_3$ and $f_4$ are hexagons since $G_1 \subset F_{60}$.

Let $h_1, h_2 \in \mathscr{H} \cap H[B_3]$ and $u_i \in V(h_i)$ $(i = 1, 2)$ as illustrated in Fig. 21(a). Let $G_2 := G_1 - \{u_1, u_3\}$ (see Fig. 21(c)). By Proposition 4.1, we have $V(\partial G_2) \subset V(\mathscr{H})$. Let $G_3 := F_{60} - (G_2 - \partial G_2)$. Then $G_3$ has six pentagons and $|G_3 \cap \mathscr{H}| = 6$. Let $f$ be the unique face of $G_3$ which is not a face of $F_{60}$. Then $G_3 \cup G_2 = F_{60}$ and $G_3 \cap G_2 = f = \partial G_2$. So a 2-degree vertex (resp. 3-degree vertex) of $G$ on $f$ is identified to a 3-degree vertex (resp. 2-degree vertex) on $\partial G_2$ in $F_{60}$.

If $B_3 \not\subseteq G_3$, then every hexagon in $G_3 \cap \mathscr{H}$ belongs to either $C[B_1]$ or $C[B_2]$. For $h_i \in G_3 \cap \mathscr{H}$ $(i = 1, 2)$, let $P_i = \partial C[B] \cap \partial G_2$ where $B = B_1$ or $B_2$. Since $F_{60}$ is cubic, $|P_i| \geq 11$ for $i = 1, 2$ (the thick paths on $\partial C[B_1]$ or $\partial C[B_2]$ connecting vertices $u$ and $v$ in Fig. 20). Therefore, $|V(f)| \geq 11 + 11 - 2 = 20$ which contradicts $|V(f)| = |V(\partial G_2)| = 16$. So $B_3 \subset G_3$. □

**Lemma 4.6.** *There are two distinct extremal fullerene graphs which have* 60 *vertices and contain $B_3$ as subgraphs.*

**Proof.** If $B_3 \subset F_{60}$, then $F_{60}$ contains two subgraphs isomorphic to $B_3$ by Lemma 4.5. Let $C[B_3]$ be the Clar extension of $B_3$ (see Fig. 22(a)). If two subgraphs isomorphic to $C[B_3]$ have common hexagons in $\mathscr{H}$, according to the proof of Lemma 4.5, the common hexagons belong to $\{h_1, h_2\}$ (see Fig. 22(a)). By the symmetry, let $h_2$ be a common hexagon. Let $f_1, f_2$ be two faces adjoining the $C[B_3]$ as shown in Fig. 22(b). Then one of $f_1$ and $f_2$ is a pentagon of the second $B_3$ since $h_2$ belongs to the Clar set of the second $C[B_3]$. If $f_1$ is a pentagon, then a fullerene graph $F_{48}$ is formed as illustrated in Fig. 22(b). If $f_2$ is a pentagon, then another fullerene graph $F_{48}$ is formed as illustrated in Fig. 22(c).

So suppose the two subgraphs isomorphic to $C[B_3]$ have no common hexagon in $\mathscr{H}$. Further, the two subgraphs isomorphic to $C[B_3]$ have no common vertex. Since $|V(C[B_3])| = 30$, hence $F_{60}$ is formed by using edges to connect the 2-degree vertices on the boundaries of the two subgraphs isomorphic to $C[B_3]$. On the other hand, the faces of $F_{60}$ do not belong to two $C[B_3]$s are hexagons. The boundary labeling of $C[B_3]$ is 33113311. Hence the 3-length degree-saturated path of one $C[B_3]$ together with the 1-length degree-saturated path of another $C[B_3]$ form a hexagon. Since the paths with same length have two distinct positions on the $\partial C[B_3]$, use the labeling $33'11'33'11'$ (see Fig. 22(a)) to distinguish the same length degree-saturated paths with different positions. If the new hexagons consist of either the paths with label 3 and the paths

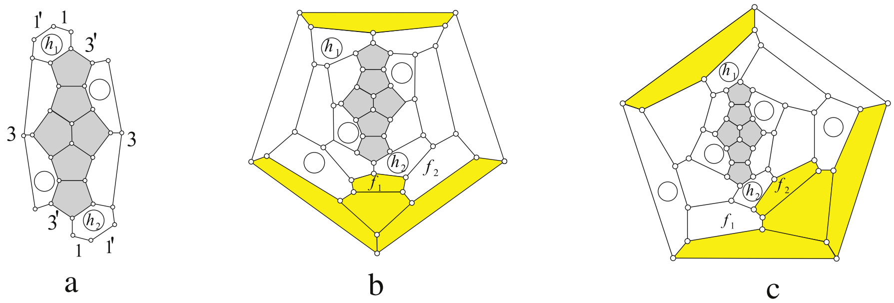


**Fig. 22.** Illustration for the proof of Lemma 4.6.

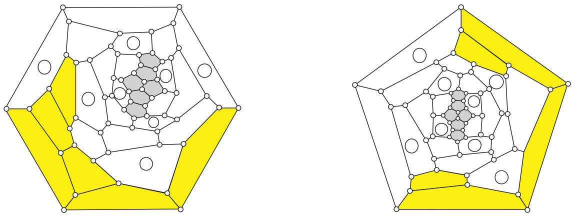

**Fig. 23.** Extremal fullerene graphs $F_{60}^1$ and $F_{60}^2$.

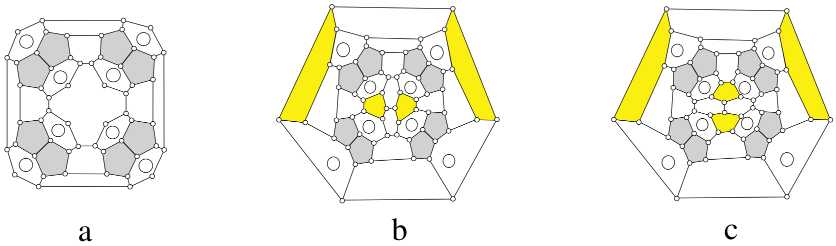


**Fig. 24.** Extremal fullerene graphs $F_{60}^3$ and $F_{60}^4$ with $B_1^4$ as maximal subgraphs.

with label 1 or the paths with label 3′ and the paths with label 1′, then a $F_{60}$ is formed as illustrated in Fig. 23 (left). If the new hexagons consists of either the paths with label 3′ and the paths with label 1 or the paths with label 3 and the paths with label 1′, then another $F_{60}$ is formed as illustrated in Fig. 23 (right). So there are exactly two extremal fullerene graphs $F_{60}^1$ and $F_{60}^2$ with $B_3$ as subgraphs. □

**Lemma 4.7.** *There are six distinct extremal fullerene graphs which have* 60 *vertices and contain* $B_1^k$ $(2 \leq k \leq 4)$ *as subgraphs.*

**Proof.** *Case* 1: $B_1^4 \subset F_{60}$ is maximal. Since $c(F_{60}) = 8$, we have that $B_1^4$ is unique and its Clar extension $C[B_1^4]$ is the graph illustrated in Fig. 24(a). By Lemma 2.2, we have two different externmal fullerene graphs $F_{60}^3$ and $F_{60}^4$ as shown in Fig. 24(b) and (c).

*Case* 2: $B_1^3 \subset F_{60}$ is maximal. There are two cases for $B_1^3$ whose Clar extensions are illustrated in Fig. 25(a) and (b). By Proposition 4.2, the graph (a) is not a subgraph of $F_{60}$. So $B_1^3 \subset F_{60}$ is unique and its Clar extension $C[B_1^3]$ is the graph (b). Let $h_1, h_2, \ldots, h_8$ be the all eight hexagons in $C[B_1^3] \cap \mathscr{H}$ and let $v, v_1, v_2, \ldots, v_7, u, u_1, u_2, \ldots, u_7$ be all 2-degree vertices on the boundary of $C[B_1^2]$ as shown in Fig. 25(b). Let $f_1$ be the face adjoining $C[B_1^2]$ (see Fig. 25(b)).

If $f_1$ adjoins three hexagons in $\mathscr{H}$, then either $v_5v_6 \in E(f_1)$ or $v_6v_7 \in E(f_1)$ by symmetry. If $v_5v_6 \in E(f_1)$, then $v$, $v_1$ are adjacent to $v_5$, $v_4$, respectively. Then, by Lemma 2.2, $v_2$ is adjacent to $v_3$. Then the edge $v_2v_3$ together with the 3-length degree-saturated path connecting $v_2$ and $v_3$ form a 4-length cycle in $F_{60}$, a contradiction. So suppose $v_6v_7 \in E(f_1)$. Then $u_1$ is adjacent to $u_7$ (see Fig. 25(c)). Let $f_2$ and $f_3$ be the two faces adjoining the graph (c). Each of $f_2$ and $f_3$ has five 2-degree vertices. Let $I[f_i]$ $(i = 2, 3)$ be the subgraph consisting of $f_i$ together with its interior. Then $I[f_2]$ and $I[f_3]$ together contain three edges in $M$. One of them, say $I[f_2]$, satisfies that $I[f_2] - f_2$ is an edge in $M$. However, the two ends of one edge are adjacent to at most four 2-degree vertices on $f_2$ since $F_{60}$ is cubic, contradicting that $f_2$ has five 2-degree vertices.

So suppose that $f_1$ contains an edge $e = w_1w_2 \in M$. By Proposition 4.1, let $f_2$ and $f_3$ be two pentagons such that $f_2 \cap f_1 = w_1u$ and $f_3 \cap f_1 = w_2v$ (see Fig. 26 (left)). According to Lemma 4.5, either $e \in E(B_2) \cap M$ or $e \in E(B_1) \cap M$. First suppose $e \in E(B_2)$. Let $f_4$ be the pentagon containing $e$ (see Fig. 26 (left)). Then one of $f_2$ and $f_3$, say $f_3$, is adjacent to two

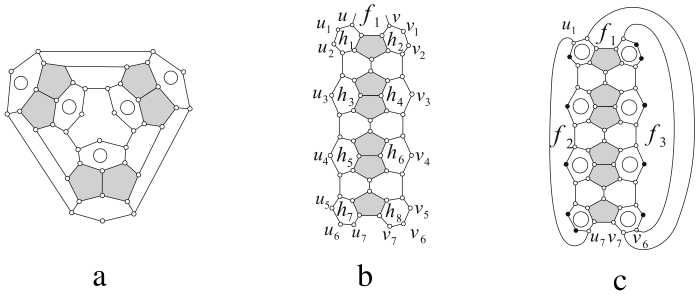


**Fig. 25.** Illustration for the proof of Case 2.

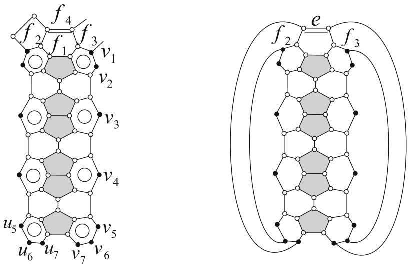


**Fig. 26.** Illustration for the proof of Case 2.

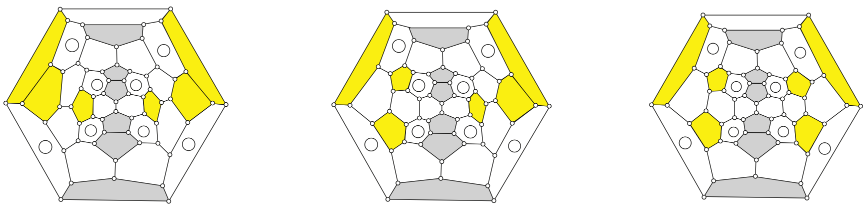

**Fig. 27.** Extremal fullerene graphs $F_{60}^5$, $F_{60}^6$ and $F_{60}^7$.

hexagons in $\mathcal{H}$. Then $f_3$ adjoins either $h_8$ or $h_7$ since $c(F_{60}) = 8$. Note that $v_6v_7 \notin E(f_2)$ and $u_5u_6 \notin E(f_3)$ since $f_4$ is a pentagon. So suppose either $v_5v_6 \in E(f_2)$ or $u_6u_7 \in E(f_2)$. If $v_5v_6 \in E(f_3)$, then $v_1$ is adjacent to $v_5$ and hence $v_2, v_3, v_4 \in V(\mathcal{H})$ are the all 2-degree vertices on a face boundary, contradicting Proposition 4.2. If $u_6u_7 \in E(f_3)$, then $v_1$ is adjacent to $u_7$ and hence $v_2, v_3$ are adjacent to $v_7, v_6$, respectively. Furthermore, $v_4$ is adjacent to $v_5$ by Lemma 2.2. Hence a subgraph of $F_{60}$ with a 4-length cycle is formed, a contradiction.

So suppose $e \in E(B_1)$. Then both $f_2$ and $f_3$ adjoin two hexagons in $\mathcal{H}$. Hence, $f_2$ and $f_3$ adjoin $h_7$ and $h_8$, respectively. Obviously, $v_6v_7 \in E(f_2)$ and $u_6u_7 \in E(f_3)$ (see Fig. 26 (right)). By Lemma 2.2, there are three distinct extremal fullerene graphs $F_{60}^5$, and $F_{60}^6$ and $F_{60}^7$ with the graph as shown in Fig. 26 (right) as a subgraph (see Fig. 27).

*Case* 3: $B_1^2 \subset F_{60}$ is maximal and $B_1^3 \not\subseteq F_{60}$. Then $|C[B_1] \cap \mathcal{H}| \geq 6$. Let $h_1, \ldots, h_6$ be the six hexagons in $C[B_1] \cap \mathcal{H}$ as illustrated in Fig. 28(a). Let $v_1, \ldots, v_7$ and $u_1, \ldots, u_7$ be the all 2-degree vertices on the $\partial C[B_1^2]$ and let $f_1, f_2$ be two hexagons adjoining $C[B_1^2]$ such that $u_1, v_1 \in V(f_1)$ and $u_7, v_7 \in V(f_2)$ (see Fig. 28(a)). Obviously, $f_1 \neq f_2$. Let $uv \in E(f_1)$, then either $uv \in M$ or $uv \in E(\mathcal{H})$.

If $uv \in M$, then either $uv \in E(B_1)$ or $uv \in E(B_2)$. By Proposition 4.1, let $f_3$ and $f_4$ be the pentagons met by $uv$ but not containing it (see Fig. 28(b)). If $uv \in E(B_1)$, by Proposition 4.2, $f_3$ does not adjoin $h_5$. If $f_3$ adjoins $h_6$, then either $v_5v_6 \in E(f_3)$ or $v_6v_7 \in E(f_3)$. If $v_5v_6 \in E(f_3)$, then $v$ is adjacent to $v_5$ and hence $v$ is adjacent to $v_4$ to bound a hexagon. Then a subgraph of $F_{60}$ is formed, which has a face with only $v_2, v_3$ connected by a 1-length degree-saturated path on its boundary, contradicting Proposition 4.2. So suppose $v_6v_7 \in E(f_3)$. Then $u_2$ is adjacent to $v_7$ and hence $u_3$ is adjacent to $u_7$. A subgraph of $F_{60}$ is formed, which has a face with only three 2-degree vertices $u_4, u_5, u_6 \in V(\mathcal{H})$, also contradicting Proposition 4.2. By symmetry, $f_4$ does not adjoin $h_5$ and $h_6$. So $f_3$ and $f_4$ adjoin the two hexagons in $\mathcal{H} \setminus \{h_1, \ldots, h_6\}$ (see Fig. 28(c)).

Let $f_5$ and $f_6$ be the faces adjoining the $B_1$ with $uv \in E(B_1)$ along its pasting edges (see Fig. 28). Since $B_1^3 \not\subseteq F_{60}$, at least one of $f_5$ and $f_6$ is a hexagon. If both $f_5$ and $f_6$ are pentagonal, then $F_{60}$ still contains a $B_1^3$ which contains three edges in $M$ as $M \cap E(f_5)$, $M \cap E(f_6)$ and $M \cap E(f_2)$ since $f_2$ is a hexagon. By symmetry, we may assume $f_5$ is a pentagon and $f_6$ is a hexagon. Then we have a graph as illustrated in Fig. 28(c) which has four 2-degree vertices on its boundary. By Lemma 2.2, there is a unique extremal fullerene graph $F_{60}^8$ which contains three subgraphs isomorphic to $B_1^2$ as maximal subgraphs (see Fig. 28(d)) since $f_2$ is hexagon. Now suppose $uv \in E(B_2)$. Let $f_5$ and $f_6$ be the faces adjoining $f_3$ and $f_4$, respectively. By symmetry, say

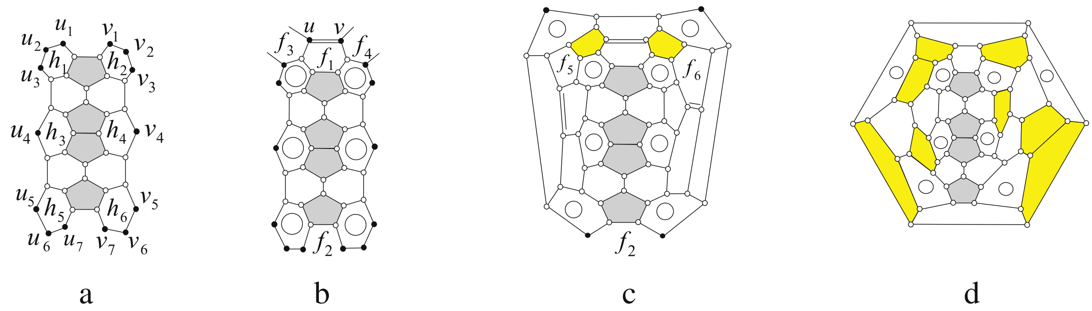


**Fig. 28.** Illustration for the proof of Case 3 and the extremal fullerene graph $F_{60}^{8}$.

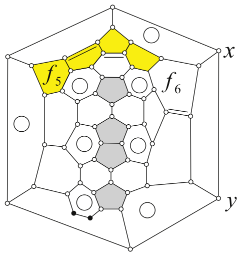


**Fig. 29.** Illustration for the proof of Case 3.

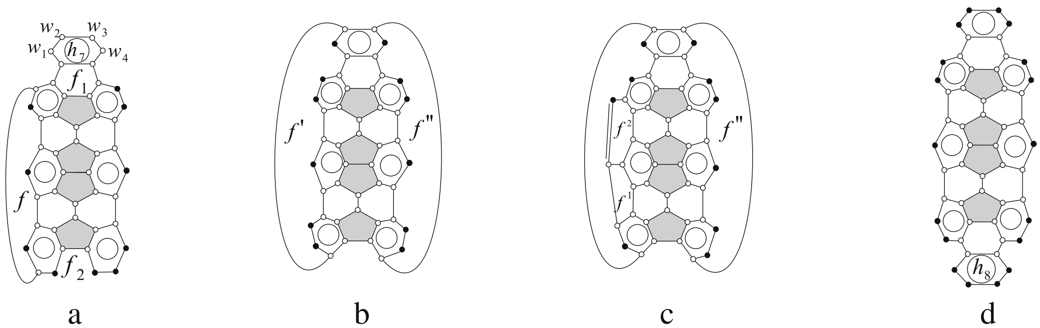


**Fig. 30.** Illustration for the proof of Case 3.

$f_5 \subset B_2$ (see Fig. 29). By Proposition 4.2, the Clar extension of the $B_2$ containing $f_5$ has two hexagons in $\mathcal{H} \setminus \{h_1, \ldots, h_6\}$. Whether $f_6$ is a hexagon or a pentagon, the vertex $x$ is adjacent to $y$ in $F_{60}$. Hence a subgraph of $F_{60}$ is formed as the graph in Fig. 29, contradicting Proposition 4.2.

So, in the following, suppose that $uv \in E(\mathcal{H})$. By Proposition 4.2, $uv \notin E(h_5)$ and $uv \notin E(h_6)$. Let $h_7 \in \mathcal{H}$ and $uv \in E(h_7)$ and let the vertices of $h_7 - uv$ be $w_1$, $w_2$, $w_3$ and $w_4$ (see Fig. 30(a)). By the symmetry of $f_1$ and $f_2$, assume $f_2$ also adjoins three hexagons in $\mathcal{H}$. Then $f_2$ adjoins only hexagons $\mathcal{H} \setminus \{h_1, h_2, \ldots, h_6\}$. If $f_2$ adjoins $h_7$, then either $w_1w_2 \in E(f_2)$ or $w_2w_3 \in E(f_2)$ by symmetry of $w_1w_2$ and $w_3w_4$. If $w_1w_2 \in E(f_2)$, then $w_1$ and $u_2$ are adjacent to $u_7$ and $u_6$, respectively. Therefore, a subgraph of $F_{60}$ with a face $f$ with three 2-degree vertices $u_3, u_4, u_5 \in V(\mathcal{H})$ is formed (see Fig. 30(a)), contradicting Proposition 4.2. So suppose $w_2w_3 \in E(f_2)$, then $w_2$ and $w_3$ are adjacent to $u_7$ and $v_7$, respectively. Let $f'$ and $f''$ be two faces as illustrated in the graph (b) in Fig. 30. By symmetry of $f'$ and $f''$, we may assume that the unique hexagon $\mathcal{H} \setminus \{h_1, h_2, \ldots, h_7\}$ lies in the $f'$. Let $I[f']$ and $O[f']$ be the subgraphs of $F_{60}$ consisting of $f'$ together with it interior and $f'$ together with its exterior, respectively. Let $f^1, f^2, f^3, f^4$ be the four faces of $F_{60}$ adjoining $O[f']$ along the four 3-length degree-saturated paths. If one of them is a pentagon, say $f^1$, then $f^1$ contains a vertex covered by one edge $e \in M$. Let $e \in E(f_2)$ (see Fig. 30(c)). Then $O[f'] \cup f^1 \cup f^2$ has a face with only four 2-degree vertices on its boundary. Note that the hexagon in $\mathcal{H} \cap I[f']$ has to lie within this face, contradicting that $c\lambda(F_{60}) = 5$. So all face of $f^i$ ($i = 1, 2, 3, 4$) are hexagons. Let $G \in \mathcal{G}_{60}$ lie within $I[f']$. Then $G$ contains or adjoins at most three hexagons in $\mathcal{H} \setminus \{h_2, h_4, h_6, h_3, h_7\}$, which contradicts that a Clar set of $H[G']$ has at least four hexagons for any $G' \in \mathcal{G}_{60}$.

So suppose $f_2$ adjoins the hexagon $h_8 \in \mathcal{H} \setminus \{h_1, h_2, \ldots, h_7\}$ (see Fig. 30(d)). Let $G''$ be the graph (d) in Fig. 30. Then $G''$ contains all hexagons in $\mathcal{H}$. So all eight vertices of $F_{60} - V(G'')$ are covered by four edges in $M$ which belong to $E(B_1)$ or $E_{(B_2)}$. That means joining some 2-degree vertices on $\partial G''$ will forming some faces with boundary labeling 3333 (corresponding to the inner face of $C[B_1] - M$ with 2-degree vertices) or 331331 (corresponding to the inner face of $C[B_2] - M$ with

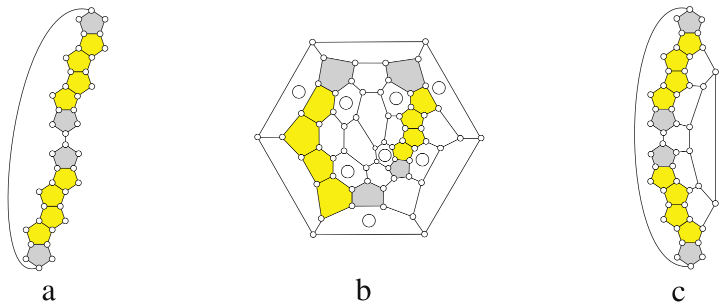


**Fig. 31.** Illustration for the proof of Case 1 and the extremal fullerene graph $F_{60}^{9}$.

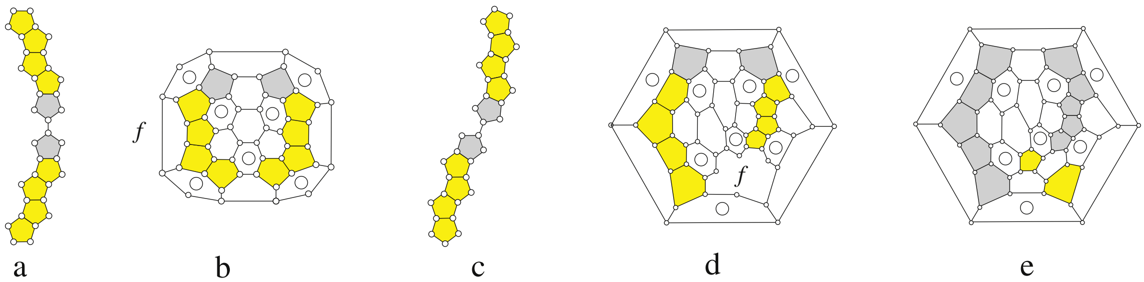


**Fig. 32.** Illustration for the proof of Case 2 and the extremal fullerene graph $F_{60}^{10}$.

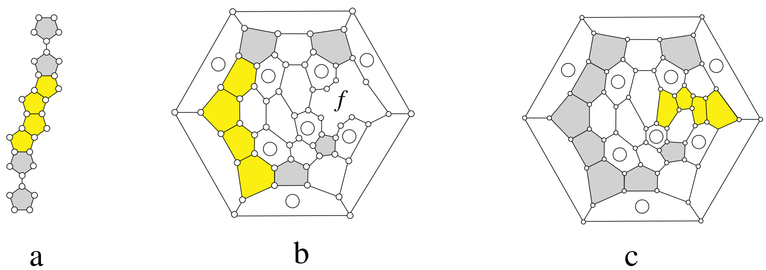


**Fig. 33.** Illustration for the proof of Case 3 and the extremal fullerene graph $F_{60}^{11}$.

2-degree vertices) (see Fig. 17). Hence the boundary labeling of $\partial G''$ should contains 13331 or 1313311 as subsequences, which contradicts the boundary labeling of $\partial G''$ is 331311131331311131. So $G'' \nsubseteq F_{60}$.

Combining Cases 1, 2 and 3, we have exact six fullerene graphs $F_{60}$ which contain $B_l^k$ $(2 \leq k \leq 4)$ as subgraphs. $\square$

**Lemma 4.8.** *There are four distinct extremal fullerene graphs $F_{60}$ such that $B_2 * B_1 \subset F_{60}$ and $B_1^k \nsubseteq F_{60}$ $(2 \leq k \leq 4)$.*

**Proof.** *Case* 1: $B_2 * B_1 * B_2 * B_1 \subset F_{60}$ is maximal. Then $B_2 * B_1 * B_2 * B_1$ has two different cases as illustrated in Fig. 31(a) and (c) since $c(F_{60}) = 8$. The Clar extension of the graph (a) induces an extremal fullerene graph $F_{60}^{9}$ as shown in Fig. 31(b). By Proposition 2.3, the graph (c) is not a subgraph of $F_{60}$. So there exists a unique $F_{60}$ containing $B_2 * B_1 * B_2 * B_1$ as a subgraph.

*Case* 2: $B_2 * B_1 * B_2 \subset F_{60}$ is maximal. By Lemma 4.3, $B_2^2 \nsubseteq F_{60}$. So $B_2 * B_1 * B_2$ has two different cases as illustrated in Fig. 32(a) and (c). Their Clar extension induces the graphs (b) and (d). Both the graphs (b) and (d) have a face $f$ with four 2-degree vertices on its boundary. By Lemma 2.2, an extremal fullerene graph containing the graph (b) has Clar number seven. So the graph (b) is not a subgraph of $F_{60}$. From the graph (d), only one fullerene graph $F_{60}^{10}$ contains $B_2 * B_1 * B_2$ as a maximal subgraph (see Fig. 32(e)).

*Case* 3: $B_1 * B_2 * B_1 \subset F_{60}$ is maximal. By the proof of Lemma 4.3, $B_1 * B_2 * B_1$ is unique as shown in Fig. 33(a). Its Clar extension induces the graph (b), which has a face $f$ with six 2-degree vertices on its boundary. So the remaining four pentagons adjoin at most four hexagons in $\mathcal{H}$ which are adjacent with $f$ in the graph (b). Hence the four pentagons belong to a $B_2$ by Lemma 4.4. So there is a unique fullerene graph $F_{60}^{11}$ contains $B_1 * B_2 * B_1$ as a maximal subgraph (see Fig. 33(c)).

*Case* 4: $B_1 * B_2 \subset F_{60}$ is maximal. Then it is unique as shown in Fig. 34(a). Let $f_1, f_2$ be two faces adjoining the Clar extension $C[B_1 * B_2]$ as shown in Fig. 34(a). Since $B_1 * B_2$ is maximal, $f_1$ and $f_2$ are two pentagons. By Proposition 4.2, $f_1$ contains an edge $e$ such that $e \notin E(C[B_1 * B_2])$ and $e \notin E(f_2)$. Clearly, $e \in M$ or $e \in E(\mathcal{H})$.

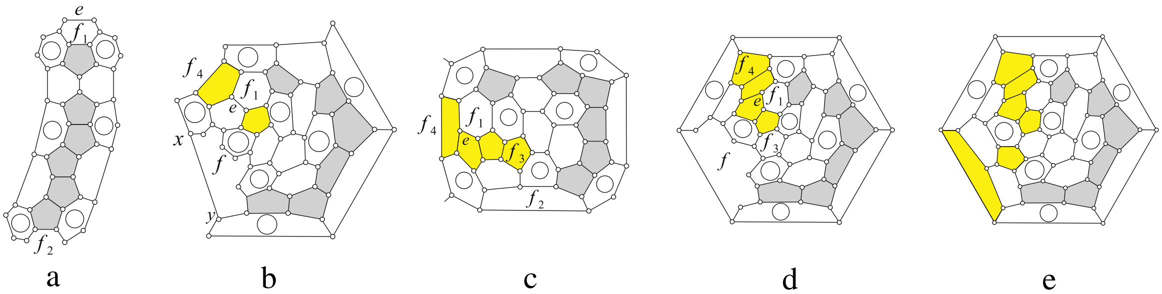


**Fig. 34.** Illustration for the proof of Subcase 4.1 and the extremal fullerene graph $F_{60}^{12}$.

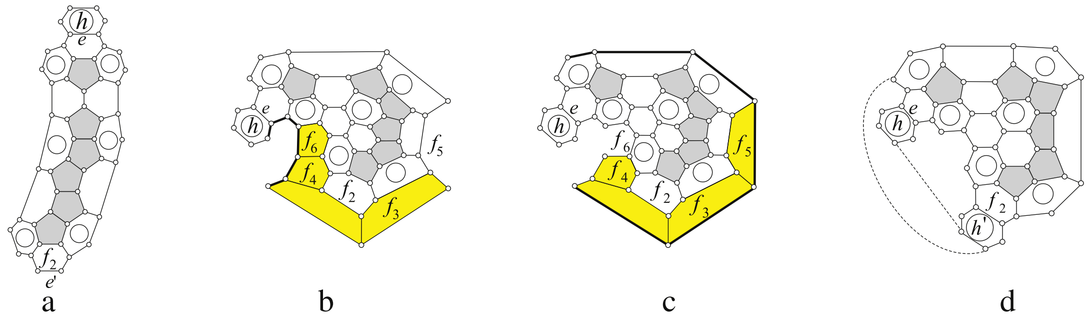


**Fig. 35.** Illustration for the proof of Subcase 4.2.

*Subcase* 4.1: $e \in M$. By Lemma 4.5, either $e \in E(B_2)$ or $e \in E(B_1)$.

If $e \in E(B_1)$, then the $B_1$ adjoins two new hexagons in $\mathscr{H}$ by Proposition 4.2. Let $x, y \in V(\mathscr{H})$ as shown in Fig. 34(b). Then the $C[B_1] \cup C[B_1 * B_2]$ is the graph (e) without the edge $xy$ in Fig. 34. Whether $f_4$ is a pentagon or a hexagon, $x$ is always adjacent to $y$. Hence, a subgraph of $F_{60}$ is formed, which has a face $f$ with four 2-degree vertices in $V(\mathscr{H})$ and with boundary labeling 5313, contradicting Proposition 4.2.

So suppose $e \in E(B_2)$. All faces meeting $e$ except $f_1$ are pentagonal. Let $f_3$ and $f_4$ be the faces adjoining $C[B_1 * B_2]$ as shown in Fig. 34(c) and (d). Then either $f_3$ is a pentagon of $B_2$ or $f_4$ is a pentagon of $B_2$. If $f_3$ is a pentagon, then the $C[B_2] \cup C[B_1 * B_2]$ is the graph (c) in Fig. 34. Since the $C[B_2] \cup C[B_1 * B_2]$ has four 2-degree vertices on its boundary and has only seven hexagons in $\mathscr{H}$, it is not a subgraph $F_{60}$ by Lemma 2.2. So suppose $f_4$ is a pentagon of the $B_2$. Then the $C[B_2] \cup C[B_1 * B_2]$ is the graph (d) in Fig. 34. By Lemma 2.2 and that $B_1 * B_2$ is maximal in $F_{60}$, there is a unique fullerene graph $F_{60}^{12}$ containing the graph (d) (see Fig. 34(e)).

*Subcase* 4.2: $e \in E(\mathscr{H})$. Let $h \in \mathscr{H}$ be the hexagon such that $e \in E(h)$. By Proposition 4.2, $f_2$ contains an edge $e'$ such that $e' \notin E(C[B_1 * B_2] \cup h)$ (see Fig. 35(a)). Then either $e' \in M$ or $e' \in E(\mathscr{H})$.

If $e' \in M$, then either $e' \in E(B_1)$ or $e' \in E(B_2)$ by Lemma 4.5. If $e' \in E(B_1)$, by Proposition 4.2, then the Clar extension $C[B_1]$ contains two hexagons in $\mathscr{H}$ which are different from the seven hexagons in $\mathscr{H} \cap (C[B_1 * B_2] \cup h)$. Further, $|\mathscr{H}| \geq 9$ contradicts $c(F_{60}) = 8$. So suppose $e' \in E(B_2)$. Let $f_3, f_4$ be the two pentagons meeting $e'$ but $e' \notin E(f_3 \cup f_4)$. Let $f_5$ and $f_6$ be two faces adjoining $f_3$ and $f_4$, respectively (see Fig. 35(b) and (c)). Whether $f_5 \subset B_2$ or $f_6 \subset B_2$, we always have a fragment with a 6-length degree-saturated path on its boundary (see Fig. 35(b) and (c), the thick paths), contradicting Proposition 2.3.

So suppose $e' \in E(\mathscr{H})$. Let $h' \in \mathscr{H}$ be the hexagon containing $e'$ and different from the seven hexagons in $C[B_1 * B_2] \cup h$. Let $G$ be the graph induced by $C[B_1 * B_2] \cup h \cup h'$ (the graph (d) in Fig. 35, without broken lines). Its boundary labeling is 33313111333111 and all 2-degree vertices on it belong to $V(\mathscr{H})$. If $G \subset F_{60}$, then the six vertices in $V(F_{60}) \setminus V(G)$ are covered by three edges in $M \setminus (M \cap E(G))$ and belong to a $B_1$ or a $B_2$ by Lemma 4.5. So joining some 2-degree vertices on the boundary of the graph (d) will from some faces with boundary labeling 3333 (corresponding to $C[B_1] - M$) or 331331 (corresponding to $C[B_2]$). That means that the boundary labeling of $\partial G$ should contain 13331 (corresponding to $C[B_1] - M$) or 1313311 (corresponding to $C[B_2] - M$) as subsequences. Clearly, 33313111333111 contains two subsequences 13331. So joining four 2-degree vertices on $\partial G$ by two edges will form two faces with boundary labeling 3333 (see Fig. 35(d), the dash edges). Hence, we have a subgraph of $F_{60}$ with a face (containing the two dash edges) which has a 7-length degree-saturated path, contradicting Proposition 2.3. So there is no $F_{60}$ containing $G$.

Combing Cases 1, 2, 3 and 4, there are four extremal fullerene graphs $F_{60}$ which contain $B_2 * B_1$ as a maximal subgraph and do not contain $B_1^k$ for $2 \leq k \leq 4$. $\square$

**Lemma 4.9.** *There are six distinct fullerene graphs $F_{60}$ such that any $B_1 \subset F_{60}$ and any $B_2 \subset F_{60}$ are maximal.*

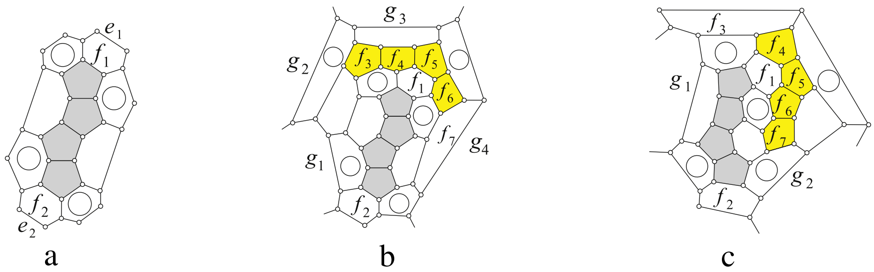


**Fig. 36.** Illustration for the proof of Case 1.

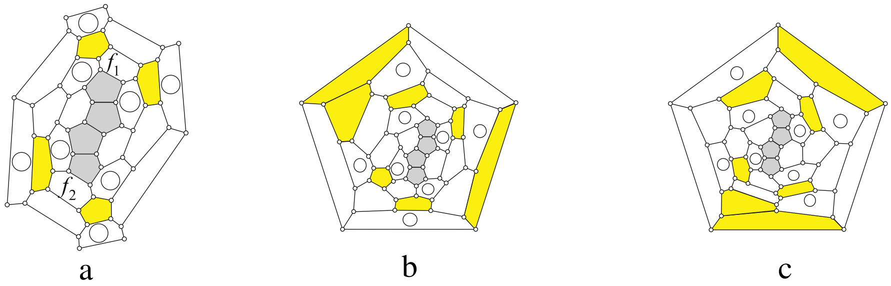


**Fig. 37.** Illustration for the proof of Case 1 and extremal fullerene graphs $F_{60}^{13}$ and $F_{60}^{14}$.

**Proof.** It is well known that $C_{60}$ is the unique fullerene graph with 60 vertices and without adjoining pentagons. So $C_{60}$ is the unique $F_{60}$ with six subgraphs isomorphic to $B_1$ as maximal subgraphs (see Fig. 1). So if $F_{60} \neq C_{60}$, then $B_2 \subset F_{60}$. Let $f_1$ and $f_2$ be the two hexagons in the hexagon extension $H[B_2]$ and let $e_i \in E(f_i)$ $(i = 1, 2)$ (see Fig. 36(a)). It is easy to see $f_1 \cap f_2 = \emptyset$ and hence $e_1 \neq e_2$. Then either $e_i \in M$ or $e_i \in E(\mathcal{H})$.

*Case* 1: $e_1, e_2 \in M$. Let $f_3, f_4, f_5, f_6$ and $f_7$ be the faces adjoining $H[B_2]$ as shown in Fig. 36(b) and (c). If $e_1$ belongs to a subgraph isomorphic to $B_2$, denote it by $B_2'$ to distinguish it from the $B_2$ in Fig. 36(a). Then either $B_2' = \cup_{i=3}^{6} f_i$ or $B_2' = \cup_{i=4}^{7} f_i$. If the former holds, then the $C[B_2] \cup C[B_2']$ induces the graph (b) in Fig. 36. Let $g_1, g_2, g_3, g_4$ be the faces adjoining $C[B_2] \cup C[B_2']$ as illustrated in Fig. 36. Note that $C[B_2] \cup C[B_2'] \cup g_1 \cup g_3 \cup g_4$ has at most four 2-degree vertices on its boundary. By Lemma 2.2, if $C[B_2] \cup C[B_2'] \subset F_n$, then $n \leq 52$. So suppose $B_2' = \cup_{i=4}^{7} f_i$. Then $f_3$ is hexagon since $B_2'$ is maximal. The $C[B_2] \cup C[B_2']$ induces the graph (c) in Fig. 36. Let $g_1, g_2$ adjoin $C[B_2] \cup C[B_2']$ as shown in Fig. 36(c). Then $C[B_2] \cup C[B_2'] \cup g_1 \cup g_2$ has at most four 2-degree vertices on its boundary. By Lemma 2.2, we have $n \leq 46$ if $C[B_2] \cup C[B_2'] \subset F_n$.

So suppose $e_1, e_2 \in E(B_1)$ by the symmetry of $e_1$ and $e_2$. Let $B_1'$ and $B_1''$ be two different subgraphs isomorphic to $B_1$ such that $e_1 \in E(B_1')$ and $e_2 \in E(B_1'')$. By Proposition 4.2, $C[B_1'] \cap C[B_1''] = \emptyset$. Hence $C[B_1'] \cup C[B_1''] \cup C[B_2]$ induces the graph (a) in Fig. 37. So the remaining four pentagons not in $C[B_1'] \cup C[B_1''] \cup C[B_2]$ adjoin at most four hexagons in $\mathcal{H}$. By Lemma 4.4, these four pentagons belong to a $B_2$. So we have two extremal fullerene graphs $F_{60}^{13}$ and $F_{60}^{14}$ (see Fig. 37(b) and (c)).

*Case* 2: $e_1 \in M$ and $e_2 \in E(\mathcal{H})$ by symmetry of $e_1$ and $e_2$. By the discussion of Case 1, we may assume $e_1 \in E(B_1) \cap M$.

Since every $B_1 \subset F_{60}$ is maximal, we have the subgraph of $F_{60}$ as illustrated in Fig. 38(a). Let $e$ be an edge on the boundary of the subgraph (a) as shown in Fig. 38(a). Then either $e \in E(\mathcal{H})$ or $e \in M$. Let $g_1, g_2, g_3$ be the faces adjoining the subgraph (a) and meeting $e$. If $e \in E(\mathcal{H})$, then $g_2 \in \mathcal{H}$. Hence we have the graph (b) in Fig. 38. If the graph (b) is a subgraph of $F_{60}$, then the remaining six pentagons not in the graph (b) adjoin at most 5 hexagons in $\mathcal{H}$, contradicting Lemma 4.4. So suppose $e \in M$. Then $g_1, g_3$ are pentagons. Then $g_2$ has to be a hexagon. Hence $e \in E(B_1) \cap M$. So we have the graph (c) in Fig. 38. Let $g_4, g_5, g_6$ and $g_7$ be the faces adjoining the subgraph (c) along 3-length degree-saturated paths. Note that the graph consisting of the graph (c) together with $g_4, \ldots, g_7$ has at most four 2-degree vertices on its boundary. Hence a fullerene graph $F_n$ containing it satisfies $n \leq 58$. So $e_1 \in M$ and $e_2 \in E(\mathcal{H})$ cannot hold simultaneously.

*Case* 3: $e_1, e_2 \in E(\mathcal{H})$. By Proposition 4.2, then $e_1$ and $e_2$ belong to two hexagons in $\mathcal{H}$ different from the hexagons in the $C[B_2]$. Let $f_3, f_4$ be two faces meeting $e_1$ and $e_2$, respectively (see Fig. 39(a)).

*Subcase* 3.1: Both of $f_3$ and $f_4$ are hexagons. Let $e_3 \in E(f_3)$ and $e_4 \in E(f_4)$. By Proposition 4.2, $e_3 \neq e_4$ and they are not edges of the graph (a) (see Fig. 39(b)).

If $e_3, e_4 \in E(\mathcal{H})$, then $e_3, e_4$ belong to two distinct hexagons in $\mathcal{H}$ and different from the hexagons in the graph (b). Hence we have the graph (c) in Fig. 39. The boundary labeling of the boundary of the graph (c) is 33113113311311 which cannot be separated into the subsequences 13331 (corresponding to $C_{B_1} - M$) and 1313311 (corresponding to $C_{B_2} - M$). So the graph (c) is not a subgraph of $F_{60}$.

So at least one of $e_3$ and $e_4$ belongs to $M$, say $e_3$. If $e_3 \in E(B_2)$, then we have the graph (a) in Fig. 40. Let $g_1$, $g_2$ and $g_3$ be the faces adjoining it as shown in Fig. 40(a). Then the graph consisting of the graph (a) together with $g_1, g_2, g_3$ and $f_4$ has at most

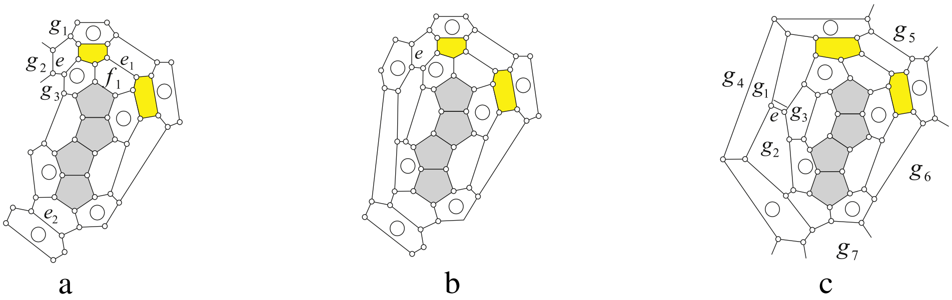


**Fig. 38.** Illustration for the proof of Case 2.

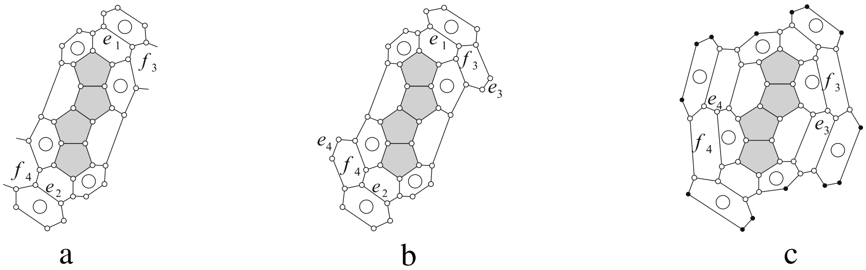


**Fig. 39.** Illustration for the proof of Case 3.1.

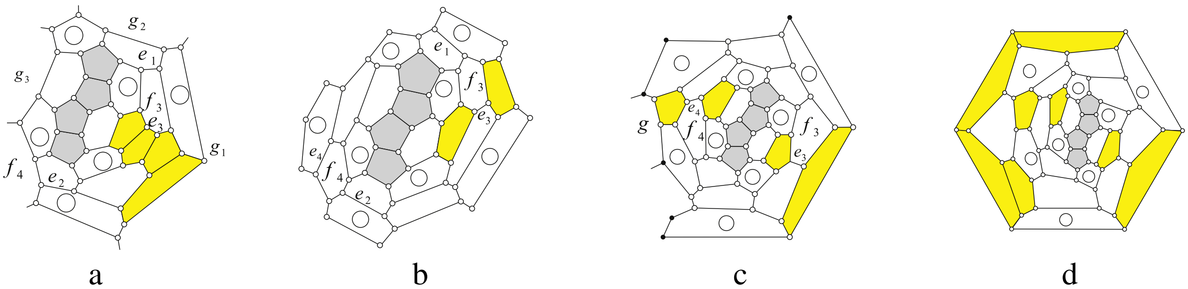


**Fig. 40.** Illustration for the proof of Case 3.1 and the extremal fullerene graph $F_{60}^{15}$.

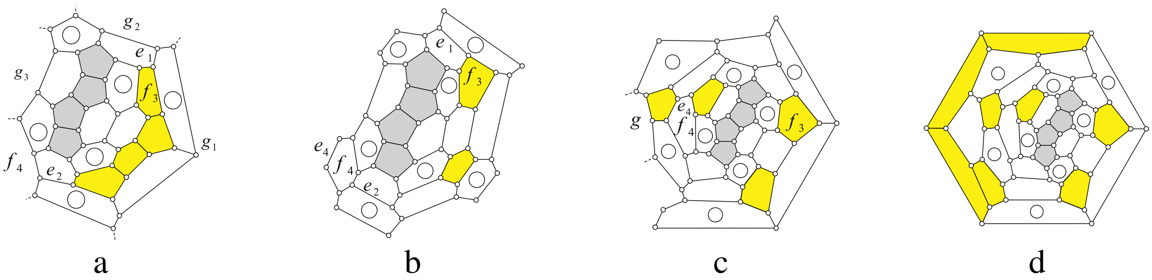


**Fig. 41.** Illustration for the proof of Subcase 3.2 and the extremal fullerene graph $F_{60}^{16}$.

four 2-degree vertices on its boundary. So a fullerene graph $F_n$ containing it satisfies that $n \leq 52$ by Lemma 2.2. So suppose $e_3 \in E(B_1)$. If $e_4 \in E(\mathscr{H})$, then we have the graph (b) in Fig. 40. If the graph (b) is a subgraph of $F_{60}$, then the remaining six pentagons not in the graph (b) adjoin at most 5 hexagons in $\mathscr{H}$, contradicting Lemma 4.4. Therefore, by the symmetry of $e_3$ and $e_4$, we may assume that $e_4 \in E(B_1) \cap M$. So we have a graph (c) in Fig. 40. Since every subgraph of isomorphic to $B_1$ or $B_2$ in $F_{60}$ are maximal, by Lemma 4.4, there is a unique extremal fullerene graph $F_{60}^{15}$ as shown in Fig. 40(d).

*Subcase* 3.2: One of $f_3$ and $f_4$ is a pentagon, say $f_3$. Let $e_4 \in E(f_4)$ as that in Subcase 3.1. If $f_3$ is a pentagon of a $B_2$, then we have the graph (a) in Fig. 41. A fullerene graph containing the graph (a) has at most 52 vertices. So suppose $f_3$ is a pentagon of a $B_1$. If $e_4 \in E(\mathscr{H})$, then we have a graph (b) in Fig. 41. As that $F_{60}$ does not contain the graph (b) in Fig. 40, the graph (b)

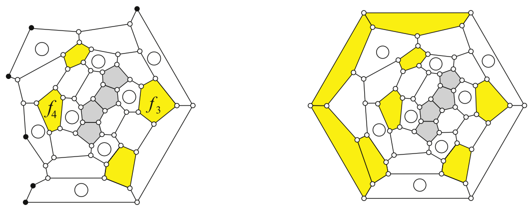


**Fig. 42.** Illustration for the proof of Subcase 3.3 and the extremal fullerene graph $F_{60}^{17}$.

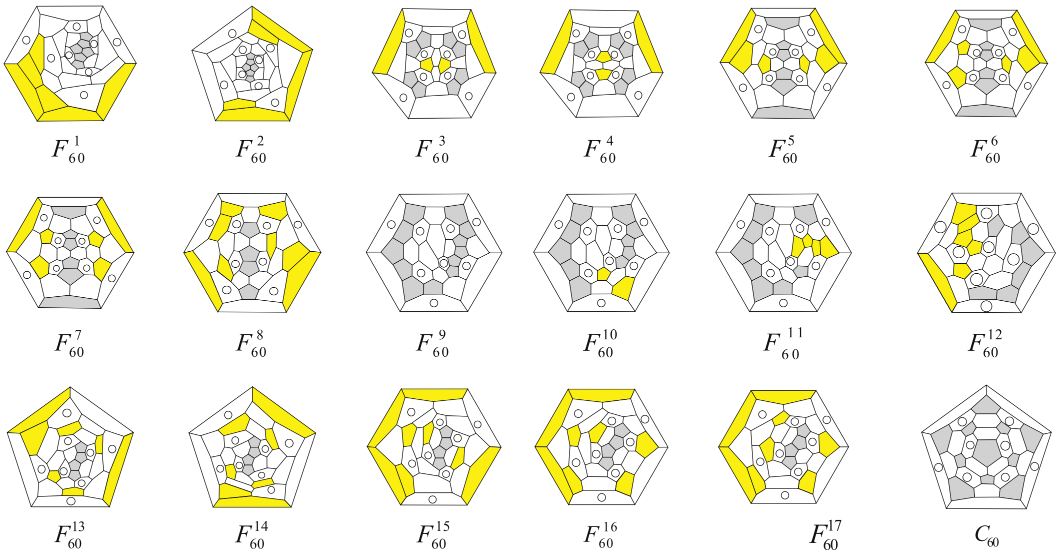


**Fig. 43.** All extremal fullerene graphs with 60 vertices.

in Fig. 41 is also not a subgraph of $F_{60}$. Hence $e_4 \in M \cap E(B_1)$. Therefore we have the graph (c) in Fig. 41. So there is a unique extremal fullerene graph $F_{60}^{16}$ containing the graph (c) since every $B_1 \subset F_{60}$ is maximal (see Fig. 41(d)).

*Subcase* 3.3: Both $f_3$ and $f_4$ are pentagonal. According to Subcase 3.2, $f_3$ and $f_4$ belong to subgraphs isomorphic to $B_1$. Hence, we have a graph as shown in Fig. 42 (left). Clearly, there are two distinct extremal fullerene graphs $F_{60}$ containing it: $F_{60}^{13}$ (the graph (b) in Fig. 37) and $F_{60}^{17}$ (the right graph in Fig. 42).

Combining Cases 1, 2 and 3, there are exact six extremal fullerene graphs $F_{60}$ such that any $B_1 \subset F_{60}$ and any $B_2 \subset F_{60}$ are maximal. □

Summarizing Lemmas 4.6–4.9, we have the following theorem:

**Theorem 4.10.** *There are exactly* 18 *distinct extremal fullerene graphs with* 60 *vertices:* $C_{60}$ *and* $F_{60}^{i}$ *for* $i = 1, 2, \ldots, 17$ *as shown in Fig.* 43.

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