

# Forcing and Anti-Forcing Numbers of (3, 6)-Fullerenes\*

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Dedicated to Professor Fujii Zhang on the occasion of his 80th birthday

## Abstract

Let  $G$  be a connected graph with at least one perfect matching. The forcing number of  $G$  is the smallest number of edges simultaneously contained in a unique perfect matching of  $G$ , denoted by  $f(G)$ . The anti-forcing number of  $G$  is the smallest number of edges whose removal from  $G$  results in a subgraph with a unique perfect matching, denoted by  $af(G)$ . In this paper, we obtain that for a (3,6)-fullerene graph  $G$ ,  $f(G) \geq 1$  and  $af(G) \geq 2$ , and any equality holds if and only if it either has connectivity 2 or is isomorphic to  $K_4$ . Further we mainly determine all the (3,6)-fullerenes with the anti-forcing number 3.

## 1 Introduction

A perfect matching of a graph coincides with a Kekulé structure in organic chemistry. Klein and Randić [9] introduced innate degree of freedom of a Kekulé structure of benzenoid graphs (or hexagonal systems), smallest number of double bonds determining the entire Kekulé structure, which plays an important role in the resonance theory in chemistry (see also [16]). Afterwards this number associated a Kekulé structure was called the forcing number of a perfect matching of a graph by Harary et al. [8]. Zhang and Li [21] determined the benzenoid graphs with a forcing edge (i.e. an edge contained in a unique

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perfect matching). Further in 1997 Li [13] determined the benzenoid graphs with a forcing single edge (i.e. anti-forcing edge). In general, Vukičević and Trinajstić [17,18] introduced the anti-forcing number of a graph as the smallest number of edges whose removal from  $G$  results in a subgraph with a unique perfect matching. Algorithms for computing the anti-forcing number of hexagonal chains and double hexagonal chains were designed by Deng [1,2].

Like the forcing number, recently Lei, Yeh and Zhang [14] proposed the anti-forcing number of any single perfect matching of a graph, showed that the forcing number of every perfect matching is no more than the anti-forcing number, and in particular showed that the maximum anti-forcing number of benzenoid graphs always equals the fries number. Klein and Rosenfeld [10] also proposed the same concept under the name “(e)-forcing”. Deng and Zhang [3] proved that the anti-forcing numbers of all perfect matchings of a cata-condensed hexagonal system form an integer interval. When considering the forcing number, the same result no longer holds. By applying  $Z$ -transformation graph (or resonance graph), Zhang and Deng [22] proved that the forcing numbers of all Kekulé structures of benzenoid graphs with a forcing edge (or the minimum forcing number one) form either the integer interval from 1 to the Clar number of  $H$  or with only the gap 2.

For  $k \geq 3$  an integer, a  $(k,6)$ -fullerene graph is a connected cubic plane (or sphere) graph whose faces are only  $k$ -gons and hexagons. The only values of  $k$  for which a  $(k,6)$ -fullerene exists are 3, 4 and 5 (see [4]). A  $(5,6)$ -fullerene is the usual fullerene as the molecular graph of sphere carbon fullerene. A  $(4,6)$ -fullerene is the molecular graph of a boron-nitrogen fullerene.

For a fullerene graph, Zhang et al. [23] showed that the minimum forcing number has at least three and this lower bound can be achieved by infinitely many fullerene graphs. Yang et al. [20] proved that a fullerene graph has the anti-forcing number at least 4. They give a procedure to construct all fullerenes whose anti-forcing numbers achieve the lower bound 4. Furthermore, they showed that, for every even  $n \geq 20$  ( $n \neq 22, 26$ ), there exists a fullerene with  $n$  vertices that has the anti-forcing number 4, and the fullerene with 26 vertices has the anti-forcing number 5. For BN-fullerene graphs (or  $(4,6)$ -fullerenes), Jiang and Zhang [11] obtained the forcing spectrum of a tubule with cyclic edge-connectivity 3. They also showed that all perfect matchings of any BN-fullerene graph have the forcing numbers at least two and constructed all seven BN-fullerene graphs with the minimum

forcing number two.

In this paper we consider the forcing number and anti-forcing number of (3,6)-fullerene graphs. The remainder is organized as follows. In Section 2, we present some basic results and preliminaries about (3,6)-fullerenes. In Section 3, we obtain that for a (3,6)-fullerene graph, its minimum forcing number is at least one and anti-forcing number is at least two, and each lower bound can be achieved if and only if it has the connectivity 2 or it is isomorphic to  $K_4$  (i.e. it is a nanotube with each end capped a pair of triangles with a common edge). In such case, by the way we show that its forcing spectrum and anti-forcing spectrum are  $\text{Spec}_f(G) = \{1, \frac{n}{4}\}$ ,  $\text{Spec}_{af}(G) = \{2, \frac{n}{4} + 1\}$  respectively, where  $n$  is the number of vertices of this graph. Further, in Section 4, we determine all the (3,6)-fullerenes with the anti-forcing number 3.

## 2 Preliminary

Let  $G$  be a simple graph with vertex set  $V(G)$  and edge set  $E(G)$ . A *perfect matching* of  $G$  is a set of edges  $M$  of  $G$  such that each vertex is incident with exactly one edge of  $M$ . A subset  $S$  of a perfect matching  $M$  of  $G$  *forces*  $M$  (or  $S$  is a forcing set of  $M$ ) if  $S$  is contained in no other perfect matching of  $G$ . The *forcing number* of  $M$ , denoted by  $f(G, M)$ , is the cardinality of a smallest set  $S$  that forces  $M$ . Let  $f(G)$  and  $F(G)$ , respectively, denote the minimum and maximum values of  $f(G, M)$  over all perfect matchings  $M$  of  $G$ . An edge is called a *forcing edge* if it is contained in a unique perfect matching of  $G$ .

For a perfect matching  $M$  of  $G$ , a subset  $S \subseteq E(G) \setminus M$  is called an *anti-forcing set* of  $M$  if  $G - S$  has a unique perfect matching  $M$ . The cardinality of a smallest anti-forcing set of  $M$  is called the *anti-forcing number* of  $M$ , denoted by  $af(G, M)$ . The anti-forcing number of  $G$  is the minimum value over anti-forcing numbers of all perfect matchings of  $G$ , denoted by  $af(G)$ . Whereas,  $Af(G) := \max\{af(G, M) : M \text{ is a perfect matching of } G\}$  is defined as the *maximum anti-forcing number* of  $G$ .

The *forcing spectrum* and *anti-forcing spectrum* of a graph  $G$  are respectively defined as  $\text{Spec}_f(G) = \{f(G, M) : M \text{ is a perfect matching of } G\}$ , and  $\text{Spec}_{af}(G) = \{af(G, M) : M \text{ is a perfect matching of } G\}$ .

For a (3,6)-fullerene  $G$ , by Euler's formula it has exactly four faces of size 3 and  $\frac{n}{2} - 2$  faces of size 6, and has the connectivity 2 or 3.

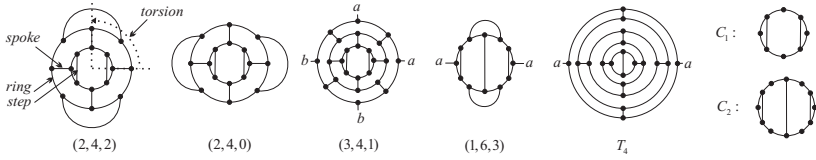


Figure 1: Five (3,6)-fullerenes and two caps  $C_1$  and  $C_2$ .

Let  $T_l$  ( $l \geq 1$ ) be the tube consisting of  $l$  cyclic chains each of two hexagons, capped on each end by a cap of two adjacent triangles. For example,  $T_4$  is depicted in Fig. 1. Note that the degenerate case  $T_0$  (i.e.  $K_4$ , the complete graph with 4 vertices) is allowed sometimes. Yang and Zhang obtained the following result.

**Theorem 2.1.** [19] *A (3,6)-fullerene  $G$  has the connectivity 2 if and only if  $G \cong T_l$  for some integer  $l \geq 1$ .*

If a (3,6)-fullerene  $G$  other than  $K_4$  has the connectivity 3, then its structure is also a tube determined only by three parameters  $r, s, t$ , where  $r \geq 1$  is the radius (number of rings),  $s$  is the size (number of spokes in each layer and  $s \geq 4$  is even) and  $t$  is the twist (torsion,  $0 \leq t \leq s$ ,  $t \equiv r \pmod{2}$ ) [5–7]. So we denote it by  $(r, s, t)$ . For example, (2, 4, 0), (2, 4, 2), (3, 4, 1), (1, 6, 3) are depicted in Fig. 1,  $C_1$  is a cap of (2, 4, 0), (2, 4, 2) and (3, 4, 1), and  $C_2$  is a cap of (1, 6, 3). In other words, a 3-connected (3,6)-fullerene  $(r, s, t)$  consists of  $r - 1$  concentric layers of hexagons (i.e. each layer is a cyclic chain of  $s$  hexagons) and two caps with torsion  $t$  on ends. If we find a cap with  $k$  steps in  $G$ , then  $G \cong (r, 2k, t)$ . This result will be applied repeatedly in Sections 4 and 5.

For a graph  $G$  with  $X \subseteq V(G)$  and  $S \subseteq E(G)$ , let  $G[X]$  and  $G[S]$  denote the subgraph of  $G$  induced by  $X$  and  $S$  respectively. Let  $e(X)$  be the number of edges in  $G[X]$ . Let  $\partial X$  be the set of edges with only one end in  $X$ . Then  $\partial X$  is an edge-cut of  $G$ . An edge-cut  $S$  of  $G$  is *trivial* if its edges are all incident with the same vertex, and *cyclic* if  $G - S$  has at least two components, each containing a cycle. A cyclic  $k$ -edge-cut is trivial if its deletion gives a cycle of length  $k$  as one component. The *cyclic edge-connectivity* of  $G$ , denoted by  $c\lambda(G)$ , is the minimum size of cyclic edge-cuts of  $G$ . We say  $G$  is cyclically  $k$ -edge-connected if  $k \leq c\lambda(G)$ .

**Lemma 2.2.** [19] *Let  $G$  be a 3-connected (3,6)-fullerene graph other than  $K_4$ . Then the four triangles of  $G$  are pairwise nonadjacent; and each triangular face of  $G$  is adjacent to*

three hexagons, both of which intersect at exactly one edge; every cyclic 3-edge-cut of  $G$  is trivial.

**Lemma 2.3.** *Suppose that  $S$  is a 3-edge-cut of a 3-connected  $(3, 6)$ -fullerene graph  $G$  other than  $K_4$ . Then  $S$  is a trivial edge-cut or a trivial cyclic 3-edge-cut of  $G$ .*

*Proof.* There exist a proper subset  $X \subset V(G)$  such that  $S = \partial X$ . Without loss of generality, assume that  $|X| \leq |\overline{X}|$ , where  $\overline{X} = V(G) \setminus X$ . Note that  $e(X) = \frac{3|X|-3}{2} = |X| + \frac{|X|-3}{2}$ . If  $S$  is not a trivial edge-cut, then  $|X| \geq 3$  since  $|X|$  is odd. So  $e(X) \geq |X|$ . This implies that  $G[X]$  and thus  $G[\overline{X}]$  each contains a cycle. That is,  $S$  is a cyclic 3-edge-cut of  $G$ . Further, By Lemma 2.2  $S$  is a trivial cyclic edge-cut.  $\square$

**Lemma 2.4.** *Let  $G$  be a 3-connected  $(3, 6)$ -fullerene graph other than  $K_4$ . Then neither 4-cycles nor 5-cycles exist in  $G$ , and each 3-cycle or 6-cycle is the boundary of a face.*

*Proof.* Since  $G$  is 3-connected, each 3-cycle bounds a face. If  $G$  has a 4-cycle  $C$ , then by Lemma 2.2  $C$  is an induced cycle of  $G$ . By definition  $C$  is not the boundary of a face. This implies that  $G$  has a 2 or 1-edge-cut, contradicting the 3-connectivity of  $G$ . Thus  $G$  has no 4-cycles. Similarly, we have that  $G$  has no 5-cycles.

Let  $C$  be a 6-cycle in  $G$ . Since  $G$  has no 4-cycles or 5-cycles,  $C$  is an induced cycle in  $G$ . We shall prove that  $C$  bounds a face of  $G$ . If not, then since  $G$  is 3-connected and  $C$  has 6 vertices,  $\partial X$  is disjoint union of two 3-edge-cuts of  $G$ , where  $X = V(C)$ , which lie outside and inside  $C$  respectively. By Lemma 2.3, any such 3-edge-cut is trivial edge-cut or trivial cyclic edge-cut of  $G$ . Either case gives the existence of 4-cycle or 5-cycle or a pair of adjacent triangles. This contradiction shows that any 6-cycle bounds a face of  $G$ .  $\square$

The following classical results are useful in our discussions.

**Theorem 2.5.** [15] *Let  $G$  be an  $r$ -regular and  $(r - 1)$ -edge-connected graph with an even number of vertices. Then the deletion of any  $r - 1$  edges of  $G$  results in a graph with a perfect matching.*

**Theorem 2.6.** [12] *Let  $G$  be a connected graph with a unique perfect matching. Then  $G$  has a cut-edge belonging to the perfect matching.*

### 3 Lower bounds for $f(G)$ and $af(G)$ of (3, 6)-fullerenes

**Lemma 3.1.** *If  $G$  is a (3, 6)-fullerene graph, then  $f(G) \geq 1$  and  $af(G) \geq 2$ .*

*Proof.* Since  $G$  is 2-connected cubic graph, Theorem 2.5 implies that each edge of  $G$  is contained in a perfect matching. So  $G$  has distinct perfect matchings and  $f(G) \geq 1$ . Further deletion of any edge of  $G$  results in a subgraph with at least two perfect matchings. So  $af(G) \geq 2$ .  $\square$

Let  $G$  be a graph with a perfect matching  $M$ . A cycle of  $G$  is  $M$ -alternating if its edges alternate in  $M$  and  $E(G) \setminus M$ . It is obvious that  $M$  is a unique perfect matching of  $G$  if and only if  $G$  has no  $M$ -alternating cycles. Let  $c(M)$  denote the maximum number of disjoint  $M$ -alternating cycles of  $G$ . A *compatible  $M$ -alternating set* of  $G$  is a set of  $M$ -alternating cycles such that any two members are either disjoint or intersect only at edges in  $M$ . Let  $c'(M)$  denote the maximum cardinality of compatible  $M$ -alternating sets of  $G$ .

**Lemma 3.2.** [14]  $f(G, M) \geq c(M)$  and  $af(G, M) \geq c'(M)$ .

Let  $M_0$  be the set of edges consisting of all spokes of a (3,6)-fullerene graph  $G$  ( $T_l$  or  $(r, s, t)$ ) and all steps in two caps. Then it is a perfect matching of  $G$ . Note that  $M_0$  is fixed in this section.

**Theorem 3.3.** *Let  $G$  be a (3, 6)-fullerene graph  $T_l, l \geq 0$ , with  $n$  vertices. Then  $\text{Spec}_f(G) = \{1, \frac{n}{4}\}$  and  $\text{Spec}_{af}(G) = \{2, \frac{n}{4} + 1\}$ .*

*Proof.* For  $T_0$ , the theorem holds obviously. Next we suppose that  $G \cong T_l, l \geq 1$ . Since each  $M_0$ -alternating cycle of  $T_l$  contains all edges of  $M_0$ , each edge in  $M_0$  is a forcing edge of  $M_0$  and any pair of adjacent edges not in  $M_0$  form an anti-forcing set of  $M_0$ . Together with Lemma 3.1 we have  $f(T_l, M_0) = 1$  and  $af(T_l, M_0) = 2$ .

For any perfect matching  $M$  of  $G$  other than  $M_0$ , it follows that  $M \cap M_0 = \emptyset$ . Clearly,  $G - M_0$  consists of  $l + 1$  concentric 4-cycles, which are disjoint  $M$ -alternating. By Lemma 3.2  $f(T_l, M) \geq l + 1 = \frac{n}{4}$ . Choosing exactly one edge of  $M$  from each concentric 4-cycle, we obtain an edge set  $S \subseteq M$ . It is obvious that  $S$  forces  $M$  and  $|S| = \frac{n}{4}$ . So  $f(G, M) = \frac{n}{4}$ .

Further,  $M \cup M_0$  forms an  $M$ -alternating cycle, denoted by  $C$ . Then  $C$  and the  $l + 1$  concentric 4-cycles of  $T_l$  form a compatible  $M$ -alternating set. By Lemma 3.2  $af(G, M) \geq c'(M) \geq l + 2 = \frac{n}{4} + 1$ . Let  $S'$  be a set of edges consisting of one edge from

$M_0$  and one edge not in  $M$  from each concentric 4-cycle. Since  $G - S'$  has no  $M$ -alternating cycles,  $S'$  is an anti-forcing set of  $M$ . Thus  $af(G, M) = \frac{n}{4} + 1$ .  $\square$

From the proof we can see that  $T_l, l \geq 1$ , has exactly  $2^{l+1} + 1$  perfect matchings, where exactly one perfect matching has forcing number 1 and anti-forcing number 2 and  $2^{l+1}$  perfect matchings have forcing number  $l + 1$  and anti-forcing number  $l + 2$ .

A *patch* of a (3, 6)-fullerene graph  $G$  is a 2-connected subgraph of  $G$  whose all interior faces are hexagons and triangles and all vertices not on the outer face have degree 3.

**Lemma 3.4.** *If  $G$  is a (3, 6)-fullerene graph other than  $T_l, l \geq 0$ , then we have*

- (i)  $G - \{v_1, v_2\}$  is 2-edge-connected for  $e = v_1v_2$  which is not an edge of a triangle;
- (ii)  $G - \{v_1, v_2, v_3, v_4\}$  is 2-edge-connected for  $\{v_1, v_2, v_3, v_4\}$  which induce  $T'$  (see Fig. 2) in  $G$ .

*Proof.* (i) Since  $G$  is a 3-connected cubic plane graph, each edge of  $G$  belongs to exactly two faces. Suppose  $e$  is shared by two hexagonal faces  $f'$  and  $f''$  of  $G$ . Let  $f_1$  and  $f_2$  be the facial cycles in  $G$  sharing exactly one endvertex of  $e$ . So  $f_1$  and  $f_2$  are disjoint. Otherwise, a nontrivial cyclic 3-edge-cut would happen, contradicting Lemma 2.2. Hence the boundary of each face in  $G - \{v_1, v_2\}$  is a cycle, and  $G - \{v_1, v_2\}$  is 2-edge-connected. (ii) Suppose that  $G[\{v_1, v_2, v_3, v_4\}] \cong T'$ . By Lemma 2.2  $G$  has patch  $B$  as shown in

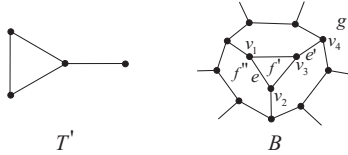


Figure 2: Illustration for the proof of Lemma 3.4.

Fig. 2. If  $g$  is a triangle, then clearly  $g$  and  $f''$  are disjoint. If  $g$  is a hexagon, then  $g$  and  $f''$  are also disjoint, otherwise,  $G$  has a nontrivial cyclic 3-edge-cut, a contradiction. So the boundary of each face in  $G - \{v_1, v_2, v_3, v_4\}$  is a cycle and  $G - \{v_1, v_2, v_3, v_4\}$  is 2-edge-connected.  $\square$

**Lemma 3.5.** *If  $G$  is a (3, 6)-fullerene graph other than  $T_l, l \geq 0$ , then  $f(G) \geq 2$ .*

*Proof.* By Lemma 3.1 it suffices to show that any edge  $e = v_1v_2$  of  $G$  cannot be a forcing edge. That is,  $G - \{v_1, v_2\}$  has at least two perfect matchings. Since  $G$  is a 3-connected

cubic plane graph, any two faces of  $G$  share at most one edge and each edge belongs to exactly two faces. Let  $f'$  and  $f''$  be distinct faces of  $G$  which share edge  $e$ .

If both  $f'$  and  $f''$  are hexagons, then  $G - \{v_1, v_2\}$  is 2-edge-connected by Lemma 3.4 and thus has at least two distinct perfect matchings by Theorem 2.6. Since  $G$  has no adjacent triangles, next we may suppose that exactly one of  $f'$  and  $f''$  is a triangle, say  $f'$ . By Lemma 2.2  $G$  has patch  $B$  as shown in Fig. 2.  $G - \{v_1, v_2, v_3, v_4\}$  is 2-edge-connected by Lemma 3.4 and has at least two distinct perfect matchings.  $\square$

The following example shows that the lower bound of Lemma 3.5 is sharp.

**Lemma 3.6.** *Let  $M$  be any perfect matching of the  $(3,6)$ -fullerene graph  $(2,4,2)$ . Then  $f(G, M) = 2$ .*

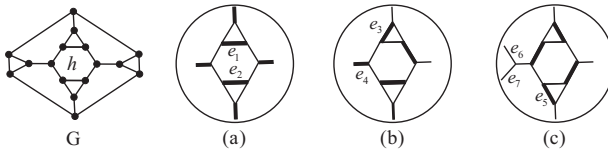


Figure 3: Illustration for the proof of Lemma 3.6 (thick edges belong to  $M$ ).

*Proof.* Let  $G$  be the  $(3,6)$ -fullerene  $(2,4,2)$  with the specific hexagon  $h$  as shown in Fig. 3. A hexagon of  $G$  is called *resonant* if it is an alternating cycle with respect to some perfect matching  $M$  of  $G$ . It is obvious that every hexagon of  $G$  is not resonant. So  $h$  has at least two vertices which is covered by the edges in  $M$  but not in  $h$ . In fact  $h$  has exactly two such vertices. By the symmetry, we only need to consider the three cases (a)-(c) in Fig. 3.

For Fig. 3(a),  $\{e_1, e_2\}$  is a forcing set of  $M$ ; For Fig. 3(b),  $\{e_3, e_4\}$  is a forcing set of  $M$ ; For Fig. 3(c),  $\{e_5, e_6\}$  or  $\{e_5, e_7\}$  is a forcing set of  $M$ . So  $f(G, M) \leq 2$ . By Lemma 3.5, we conclude that  $f(G, M) = 2$ .  $\square$

For a  $(3,6)$ -fullerene graph  $G$  other than  $T_l$ , we have  $af(G) \geq 2$ . The following result will show that the anti-forcing number has a larger lower bound.

**Lemma 3.7.** *If  $G$  is a  $(3,6)$ -fullerene graph other than  $T_l$ ,  $l \geq 0$ , then  $af(G) \geq 3$ .*



*Proof.* Suppose to the contrary that  $G$  has an anti-forcing set  $S = \{e_1, e_2\}$ . Let  $M$  be a unique perfect matching of  $G - S$ . Then  $G - S$  is connected and has a cut-edge  $e$  in  $M$  by Theorem 2.6. So  $S' := \{e_1, e_2, e\}$  is an edge-cut of  $G$ . We only need to consider the following two cases by Lemma 2.3:

*Case 1:*  $S'$  is a trivial edge-cut of  $G$ . Since  $f(G) \geq 2$  by Lemma 3.5, single edge  $e$  is contained in at least two perfect matchings  $M_1$  and  $M_2$  of  $G$ . Since  $e_1$  and  $e_2$  are adjacent to  $e$ , neither  $e_1$  nor  $e_2$  belong to  $M_1$  (resp.  $M_2$ ). So  $M_1$  and  $M_2$  are two perfect matchings of  $G - S$ , contradicting that  $S$  is an anti-forcing set of  $G$ .

*Case 2:*  $S'$  is a trivial cyclic 3-edge-cut of  $G$ . Let  $e_3$  be the edge in a triangle which is adjacent to both  $e_1$  and  $e_2$ . Then  $e_1, e_2 \notin M$  and  $e \in M$  imply that  $e_3 \in M$ . By Lemma 3.5, we can find at least two distinct perfect matchings  $M_3$  and  $M_4$  of  $G$  such that  $e_3$  belongs to both  $M_3$  and  $M_4$ . So  $e_1, e_2 \notin M_i, i = 3, 4$ . That is,  $M_3$  and  $M_4$  are two distinct perfect matchings of  $G - S$ , a contradiction.  $\square$

In summary, by Theorem 3.3 and Lemmas 3.7 and 3.5 we obtain the following theorem.

**Theorem 3.8.** *Let  $G$  be a (3,6)-fullerene graph. Then the following statements are equivalent: (i)  $f(G) = 1$ , (ii)  $af(G) = 2$ , and (iii)  $G \cong T_l$  for some integer  $l \geq 0$ .*

## 4 All (3,6)-fullerenes with the anti-forcing number 3

In this section we mainly determine all the (3,6)-fullerenes with the anti-forcing number 3. At first we describe the structure of a minimum anti-forcing set as follows.

**Lemma 4.1.** *Let  $G$  be a 3-connected (3,6)-fullerene graph other than  $K_4$  and  $S = \{e_1, e_2, e_3\}$  be an anti-forcing set. Then  $G[S]$  is neither a triangle nor star  $K_{1,3}$ .*

*Proof.* Since  $G[S]$  is not isomorphic to star  $K_{1,3}$ , it suffices to show that it is not a triangle. We can check that  $(2, 4, 0)$ ,  $(2, 4, 2)$  and  $(1, 6, 3)$  has no such anti-forcing set (see Fig. 1). Next, we consider other (3,6)-fullerenes. Let  $M$  be a unique perfect matching of  $G - S$ .

If  $G[S]$  is a triangle, then  $G$  has patch  $P_1$  as shown in Fig. 4, and  $\{u_1v_1, u_2v_2, u_3v_3\} \subset M$ . If  $f_1, f_2$  and  $f_3$  are pairwise disjoint faces, then  $G - \{u_1, v_1, u_2, v_2, u_3, v_3\}$  is 2-edge-connected since each face is bounded by a cycle, and has more than one perfect matchings by Theorem 2.6, a contradiction. So suppose that  $f_1$  and  $f_2$  share one edge. Then  $G$  has patch  $P_2$ . So  $G \cong (r, 4, t)$ ,  $r \geq 3$  (for  $r = 2$ ,  $G$  is either  $(2, 4, 0)$  or  $(2, 4, 2)$ ),

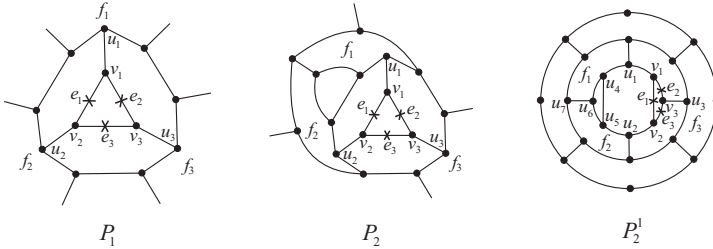


Figure 4: Illustration for the proof of Theorem 4.1.

and  $G$  has patch  $P_2^l$ . Further,  $\{u_1v_1, u_2v_2, u_3v_3, u_4u_5, u_6u_7\} \subset M$ . We can check that  $G - \{u_1, v_1, u_2, v_2, u_3, v_3, u_4, u_5, u_6, u_7\}$  is 2-edge-connected and thus has more than one perfect matchings. A contradiction would occur.  $\square$

**Lemma 4.2.** *Let  $G$  be a 3-connected  $(3, 6)$ -fullerene graph. Then  $G$  has subgraph  $T$  as shown in Fig. 5 if and only if for some positive integer  $k$ ,  $G$  is isomorphic to either  $(2, s, 0)$ ,  $s = 2k \geq 4$ , or  $(1, s, 3)$ ,  $s = 2k \geq 8$ , or  $(1, s, \frac{s}{2})$ ,  $s = 4k + 2 \geq 6$ .*

*Proof.* It is sufficient to show the necessity. Since  $G$  is a 3-connected  $(3, 6)$ -fullerene graph,  $G \cong (r, s, t)$ , where  $r \geq 1$ ,  $s = 2k \geq 4$ ,  $t \equiv r \pmod{2}$  and  $0 \leq t \leq \frac{s}{2}$ . So  $G$  has the cap as shown in Fig. 5, the length of the cycle  $C_1$  is at least 8, and the distance between  $v_i$  and  $u_i$  on  $C_1$  is at least 2 for  $i = 1$  or 3. If  $v_2$  is adjacent to  $u_2$ , then

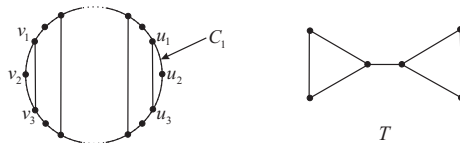


Figure 5: Illustration for the proof of Lemma 4.2.

$|V(G)| = 2rs = 2s = 2 + 2 \times (4k + 1)$  and  $G \cong (1, s, \frac{s}{2})$ ,  $s = 4k + 2 \geq 6$ . If  $v_2$  and  $u_2$  are not adjacent, then by the 3-connectivity of  $G$ ,  $G \cong (1, s, 3)$ ,  $s = 2k \geq 8$  or  $(2, s, 0)$ ,  $s = 2k \geq 4$ .  $\square$

Now, we obtain the following main result in this paper.

**Theorem 4.3.** *Let  $G$  be a  $(3, 6)$ -fullerene graph. Then  $af(G) = 3$  if and only if  $G$  is isomorphic to  $(2, s, 0)$ ,  $s = 2k \geq 4$ , or  $(1, s, 3)$ ,  $s = 2k \geq 8$ , or  $(1, s, \frac{s}{2})$ ,  $s = 4k + 2 \geq 6$ , or  $(2, 4, 2)$ , or  $(3, 4, 1)$ .*

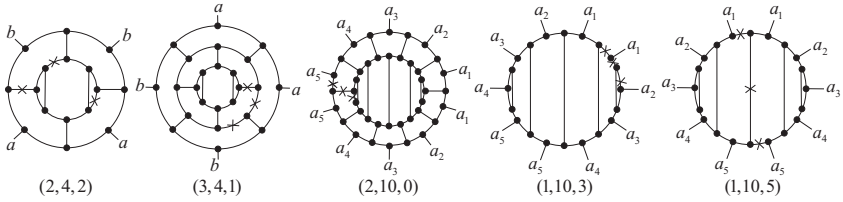


Figure 6: Five (3,6)-fullerene graphs with the anti-forcing number 3.

*Proof.* We first consider the sufficiency. For such graph  $G$ ,  $af(G) \geq 3$  by Theorem 3.8. If  $G \cong (2, 4, 2)$  or  $(3, 4, 1)$ , then  $G$  has an anti-forcing set of 3 edges, marked by crosses as shown in Fig. 6. For the other three cases, each of such three graphs has an anti-forcing set of size 3 (for example, see Fig. 6 in case  $s = 10$ ). Hence  $af(G) = 3$ .

Conversely, by Theorem 3.8 suppose that  $G$  is 3-connected and is not isomorphic to  $K_4$  and  $S = \{e_1, e_2, e_3\}$  is an anti-forcing set of  $G$ . Then it follows that  $G - S$  is connected. Let  $M$  be a unique perfect matching of  $G - S$ . By Theorem 2.6  $G - S$  has a cut-edge  $e = v_1v_2$  in  $M$ . Let  $G_1$  and  $G_2$  be the two components of  $G - S \cup \{e\}$  with  $|V(G_1)| \leq |V(G_2)|$ ,  $v_i \in V(G_i), i = 1, 2$ .

Since  $G_1$  has odd number of vertices,  $S' = S \cup \{e\}$  contains properly a 3-edge-cut of  $G$ , say  $\{e_1, e_2, e\}$ . By Lemma 2.3  $\{e_1, e_2, e\}$  is a trivial edge-cut or a trivial cyclic 3-edge-cut of  $G$ . The remaining proof is based on the following two lemmas.

**Lemma 4.4.** *If  $\{e_1, e_2, e\}$  is a trivial cyclic 3-edge-cut of  $G$ , then  $G$  has subgraph  $T$  or  $G \cong (2, 4, 2)$ .*

**Lemma 4.5.** *If  $\{e_1, e_2, e\}$  is a trivial edge-cut of  $G$ , then  $G$  has subgraph  $T$ , or  $G \cong (2, 4, 2)$  or  $(3, 4, 1)$ .*

By Lemmas 4.4 and 4.5, the necessary holds. □

Next, we prove Lemma 4.4, but the proof of Lemma 4.5 is tedious and put in the final section.

*Proof of Lemma 4.4.* By Lemma 2.2 the four triangles of  $G$  are pairwise nonadjacent, so  $G$  has at least 12 vertices and  $|V(G_2)| \geq 6$ . Suppose that  $\{e_1, e_2, e\}$  is a trivial cyclic 3-edge-cut of  $G$ . Then  $G[V(G_1)]$  is a triangle, and  $G$  has patch  $A$  (see Fig. 7) by Lemma 2.2. So  $\{v_3v_4, e\} \subset M$ . Further,  $e_3 \in G - \{v_1, v_2, v_3, v_4\}$ , otherwise,  $G - \{v_1, v_2, v_3, v_4\}$  is 2-edge-connected by Lemma 3.4 and has at least two perfect matchings, a contradiction.

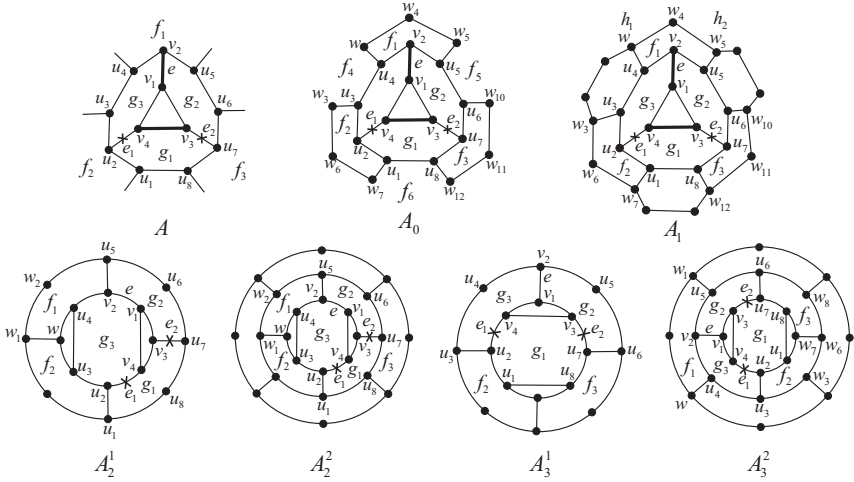


Figure 7: Illustration for the proof of Lemma 4.4.

Hence  $G_2 - v_2 = G - \{v_1, v_2, v_3, v_4\} - e_3$  is connected and has a unique perfect matching  $M_0 = M|_{G_2 - v_2}$ . So it has a cut-edge  $e'$  in  $M_0$ . The two connected components of  $G_2 - v_2 - e'$  are denoted by  $G'_1$  and  $G'_2$ . Then  $\{e', e_3\}$  is an edge-cut of  $G - \{v_1, v_2, v_3, v_4\}$ . For a subgraph  $H$  of  $G$ ,  $\partial_G(H)$  denotes a set of edges each of which has exactly one endvertex in  $H$ . We may assume that  $|\partial_G(G'_1)| = 3$  and  $|\partial_G(G'_2)| = 5$  since  $|\partial_G(G'_1)|$  and  $|\partial_G(G'_2)|$  are odd,  $|\partial_G(G'_1)| + |\partial_G(G'_2)| = 8$ , and  $|\partial_G(G'_i)| \geq 3$  by the 3-connectivity of  $G$ ,  $i = 1, 2$ . Then  $\partial_G(G'_1) = \{e_3, e', a\}$ , where  $a \in \{e_1, e_2, v_2u_4, v_2u_5\}$ . By Lemma 2.3  $\{e_3, e', a\}$  is a trivial edge-cut or a trivial cyclic 3-edge-cut of  $G$ .

Now, we suppose that  $G$  does not contain subgraph  $T$ . Then  $f_1, f_2$  and  $f_3$  are hexagons.

If  $f_1, f_2$  and  $f_3$  are mutually disjoint, then  $G$  has patch  $A_0$ , and  $f_4, f_5$  and  $f_6$  are distinct hexagons (see Fig. 7). It follows that  $f_4$  and  $f_3$  are disjoint. Otherwise, the shared edge is either  $w_{12}w_{11}$  or  $w_{11}w_{10}$ . Further, either  $w_3w_{12} \in E(G)$  or  $ww_{10} \in E(G)$ . So  $G$  has a 6-cycle which is not the boundary of a face, a contradiction by Lemma 2.4. So the other two vertices on  $f_4$  are not in  $V(A_0)$ . Similarly,  $f_6$  is disjoint with  $f_1$  and  $f_4$ , otherwise,  $G$  has 4-cycle or 6-cycle which is not the boundary of a face, and a contradiction occurs again. So  $f_6$  has two vertices in  $V(G) - V(A_0) \cup V(f_4)$ . Further,  $f_5$  has two vertices in  $V(G) - V(A_0) \cup V(f_4) \cup V(f_6)$ . Then  $G$  has patch  $A_1$ . So  $\{e_3, e', a\}$  is a trivial edge-cut and  $e_3 \in \{u_4w, u_4u_3, u_2u_1, u_2u_3, u_7u_8, u_7u_6, u_5u_6, u_5u_5\}$ . For each case of  $e_3$ , we can show

that  $G - S$  has at least two perfect matchings, a contradiction. Here, we take  $e_3 = u_1u_2$  as an example. Then  $\{v_3v_4, e, u_3u_2, u_4w\} \subset M$ ,  $G - \{v_3, v_4, v_1, v_2, u_3, u_2, u_4, w\}$  is 2-edge-connected since each face is bounded by a cycle and has more than one perfect matchings by Theorem 2.6, a contradiction.

If  $f_1$  and  $f_2$  share one edge, then  $G$  has patch  $A_2^1$ . So  $G \cong (r, 4, t)$ ,  $r \geq 2$ . If  $r = 2$ , then  $G \cong (2, 4, 2)$ . For  $r \geq 3$ ,  $G$  has patch  $A_2^2$ . Now,  $e_3 \in \{wv_1, wu_4, u_4u_3, u_5w_2, u_5u_6, u_7u_6, u_7u_8, u_2u_1, u_2u_3\}$ . For each case of  $e_3$ , we can confirm that  $G - S$  has more than one perfect matchings, a contradiction. For the case that  $f_1$  and  $f_3$  share one edge, the analogous arguments as above can be implemented.

If  $f_2$  and  $f_3$  share one edge,  $G$  has patch  $A_3^1$ . So  $G \cong (r, 4, t)$ ,  $r \geq 2$ . If  $r = 2$ , then  $G \cong (2, 4, 2)$ . For  $r \geq 3$ ,  $G$  has patch  $A_3^2$ , and  $e_3 \in \{u_5w_1, u_5u_6, u_7u_6, u_7u_8, u_2u_1, u_2u_3, u_4u_3, u_4w\}$ . We can conclude a similar contradiction for each case of  $e_3$ . ■

### 5 Proof of Lemma 4.5

Suppose that  $\{e_1, e_2, e\}$  is a trivial edge-cut of  $G$ . Then  $G_1$  is a single vertex  $v_1$ . If exactly one of two faces sharing edge  $e$  is a triangle, then  $G$  has patch  $B$  as shown in Fig. 8. Since  $S$  and  $\{v_2u_1, e_2, e_3\}$  anti-force the same perfect matching  $M$ , we can demonstrate that  $G$  has subgraph  $T$  or  $G \cong (2, 4, 2)$  by Lemma 4.4.

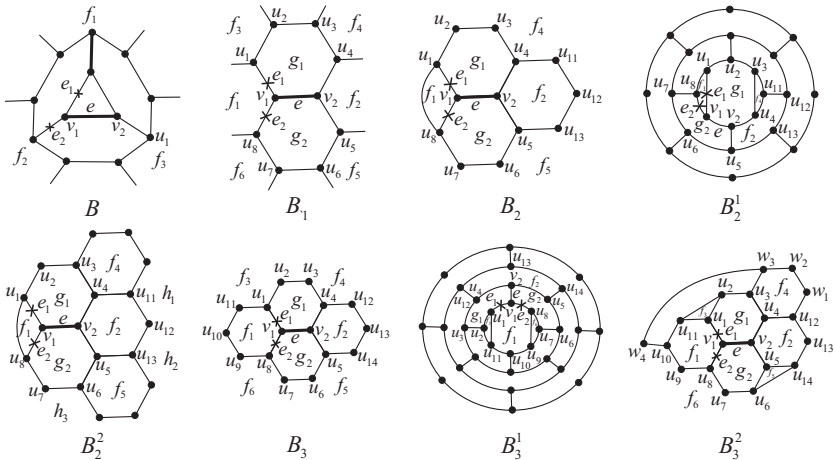


Figure 8: Illustration for the proof of Lemma 4.5 (I).

Now we suppose that the two faces sharing edge  $e$  are hexagons. Then  $G$  has patch  $B_1$  as shown in Fig. 8. Since  $G - \{v_1, v_2\}$  is 2-edge-connected by Lemma 3.4,  $e_3 \in G - \{v_1, v_2\}$  and  $G' := G - \{v_1, v_2\} - e_3$  is connected and has a unique perfect matching  $M \setminus \{e\}$ . By Theorem 2.6  $G'$  has a cut-edge  $e'$  in  $M \setminus \{e\}$ . So  $\{e_3, e'\}$  is an edge-cut of  $G - \{v_1, v_2\}$ . By analogous argument as in the proof of Lemma 4.4,  $\{e_3, e', b\}$  is a trivial edge-cut or a trivial cyclic edge-cut of  $G$ , where  $b \in \{e_1, e_2, v_2u_4, v_2u_5\}$ . We need a larger patch for considering  $e_3$ . In the following we suppose that  $G$  does not contain subgraph  $T$ . Then at most one of  $f_1$  and  $f_2$  is a triangle.

Firstly, we presume that exactly one of  $f_1$  and  $f_2$  is a triangle, say  $f_1$ . Then  $G$  has patch  $B_2$ . By Lemma 3.4  $G - \{v_1, v_2, u_1, u_8\}$  is 2-edge-connected, so  $e_3 \notin \{u_1u_2, u_7u_8\}$ . By Lemma 4.1,  $e_3 \neq u_1u_8$ . Hence  $e_3 \in G - \{v_1, v_2, u_1, u_8\}$ . If  $f_4$  or  $f_5$  is a triangle, then  $G \cong (r, 4, t)$ ,  $r \geq 2$ . For  $r = 2$ ,  $G \cong (2, 4, 2)$ . For  $r \geq 3$ ,  $G$  has patch  $B_2^1$ . So  $e_3 \in \{u_2u_3, u_3u_4, u_4u_{11}, u_5u_6, u_5u_{13}, u_{11}u_{12}\}$ . For each case of  $e_3$ ,  $G - S$  has at least two perfect matchings, a contradiction. So we may suppose that both  $f_4$  and  $f_5$  are hexagons. Then  $G$  has patch  $B_2^2$  and  $e_3 \in \{u_3u_4, u_4u_{11}, u_5u_6, u_5u_{13}\}$ . We can verify that  $G - S$  has at least two perfect matchings for each case of  $e_3$ , a contradiction.

Next, we suppose that both  $f_1$  and  $f_2$  are hexagons. Then  $G$  has patch  $B_3$  as shown in Fig. 8. Note that  $f_3, f_4, f_5$  and  $f_6$  are distinct faces, and at most one of  $f_3$  and  $f_4$  (resp.  $f_5$  and  $f_6$ ) is a triangle. Since  $S$  and  $\{v_2u_4, v_2u_5, e_3\}$  anti-force the same perfect matching  $M$ , it is sufficient to consider the following four cases.

*Case 1:* Both  $f_3$  and  $f_6$  are triangles. Then  $e_3 \in \{u_1u_{11}, u_1u_2, u_2u_3, u_3u_4, u_4u_{12}, u_5u_{14}, u_5u_6, u_6u_7, u_8u_7, u_8u_9, u_9u_{10}, u_{10}u_{11}\}$  and  $G \cong (r, 4, t)$ ,  $r \geq 3$ . For  $r = 3$ ,  $G \cong (3, 4, 1)$ . For  $r \geq 4$ ,  $G$  has patch  $B_3^1$ . Then  $G - S$  has at least two perfect matchings for each case of  $e_3$ , a contradiction.

*Case 2:* Both  $f_3$  and  $f_5$  are triangles. Then  $e_3 \in \{u_{10}u_{11}, u_1u_{11}, u_1u_2, u_2u_3, u_3u_4, u_4u_{12}, u_{13}u_{14}, u_5u_{14}, u_5u_6, u_6u_7, u_8u_7, u_8u_9\}$  and  $G$  has patch  $B_3^2$ . Since  $G$  does not contain subgraph  $T$ ,  $w_4u_9 \notin E(G)$ . So  $f_4$  and  $f_6$  are disjoint, and  $G$  has patch  $B_3^{2,1}$  (see Fig. 9). If  $f_7$  and  $f_6$  share an edge, i.e.  $w_5w_6$ , then  $w_6w_8 \in E(G)$ ,  $w_2w_4 \in E(G)$  and  $G \cong (3, 4, 1)$ . If  $f_7$  and  $f_6$  are disjoint, then  $G$  has patch  $B_3^{2,2}$ . The similar contradiction occurs for each case of  $e_3$ .

*Case 3:*  $f_3$  is a triangle, and  $f_4, f_5$  and  $f_6$  are hexagons. Then  $e_3 \in \{u_1u_2, u_2u_3, u_3u_4, u_4u_{12}, u_5u_{14}, u_5u_6, u_7u_8, u_8u_9, u_1u_{11}, u_{10}u_{11}\}$ .  $f_4$  and  $f_5$  are disjoint, so  $G$  has patch  $B_3^3$ . Since

$G$  does not contain subgraph  $T$ ,  $w_4u_9 \notin E(G)$ . So  $f_4$  and  $f_6$  are disjoint.

If  $f_5$  and  $f_6$  share an edge, then  $G$  has patch  $B_3^{3,1}$ . We assume that  $h_3$  and  $f_4$  are disjoint, otherwise,  $w_2w_4$ ,  $w_1w_8$  and  $w_5u_{13}$  are edges of  $G$  and  $G \cong (3, 4, 1)$ . Further  $h_3$  and  $f_2$  are disjoint since  $h_3$ ,  $h_1$  and  $h_2$  are distinct faces of  $G$ . So each face of  $G - \{v_1, v_2, u_8, u_9\}$  is bounded by a cycle, and thus  $G - \{v_1, v_2, u_8, u_9\}$  is 2-edge-connected. For  $e_3 = u_7u_8$ ,  $\{e, u_8u_9\} \subset M$ , so  $G - \{v_1, v_2, u_8, u_9\}$  and then  $G - S$  has at least two perfect matchings, a contradiction. The similar contradiction would occur for  $e_3 \in \{u_5u_6, u_3u_4, u_4u_{12}, u_1u_2, u_{10}u_{11}, u_1u_{11}, u_2u_3, u_8u_9, u_5u_{14}\}$ .

If  $f_5$  and  $f_6$  are disjoint, then  $G$  has patch  $B_3^{3,2}$ . If  $h_3$  and  $f_4$  are disjoint, then  $G - S$  has at least two perfect matchings for each case of  $e_3$ . If  $h_3$  and  $f_4$  share an edge, then  $w_2w_4 \in E(G)$  and  $G \cong (r, 4, t)$ ,  $r \geq 4$ . We always obtain similar contradiction for each case of  $e_3$ .

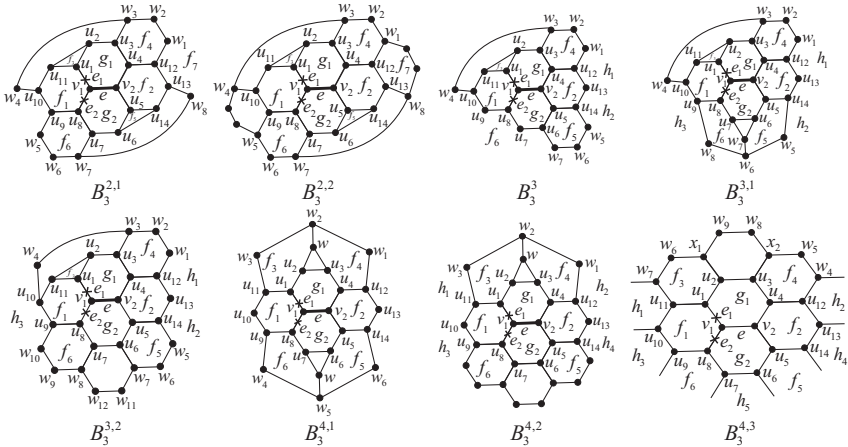


Figure 9: Illustration for the proof of Lemma 4.5 (II).

Case 4:  $f_3$ ,  $f_4$ ,  $f_5$  and  $f_6$  are hexagons. Then  $e_3 \in \{u_1u_2, u_1u_{11}, u_4u_3, u_4u_{12}, u_5u_{14}, u_5u_6, u_8u_7, u_8u_9\}$ .

If  $f_3$  and  $f_4$  share an edge, and  $f_5$  and  $f_6$  share an edge, then  $G$  has patch  $B_3^{4,1}$  and  $G \cong (r, 6, t)$ ,  $r \geq 2$ . For  $r = 2$ ,  $G \cong (2, 6, 2)$  or  $(2, 6, 0)$ . In fact  $(2, 6, 2) \cong (3, 4, 1)$  and  $(2, 6, 0)$  has subgraph  $T$ . For  $r \geq 3$ ,  $G - S$  has more than one perfect matchings for each case of  $e_3$ , a contradiction.

If  $f_3$  and  $f_4$  share an edge, and  $f_5$  and  $f_6$  are disjoint, then  $G$  has patch  $B_3^{4,2}$ . Since  $G$

does not contain subgraph  $T$ ,  $h_1$  and  $h_2$  are distinct faces of  $G$ . So  $u_{10}u_{13} \notin E(G)$ , and  $h_3$  and  $h_4$  are distinct faces. Further  $h_1$  is different from  $h_4$ , and  $h_2$  is different from  $h_3$  since  $G$  has no 5-cycles by Lemma 2.4. For each case of  $e_3$ , we can show that  $S$  does not anti-force  $M$ .

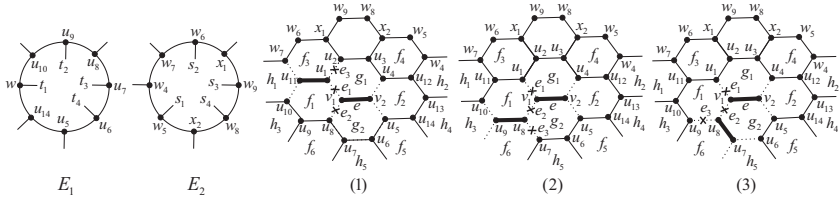


Figure 10: Edge-cuts  $E_1$  and  $E_2$ , and some cases of  $e_3$  in patch  $B_3^{4,3}$ .

Now, we consider the remaining case:  $f_3$  and  $f_4$  are disjoint, and  $f_5$  and  $f_6$  are disjoint. Then  $G$  has patch  $B_3^{4,3}$  as shown in Fig. 9. We claim that  $h_1$  is not  $h_4$  or  $h_2$ , and  $h_3$  is not  $h_4$ . Suppose that  $h_1 = h_4$ . Then  $w_7u_{13} \in E(G)$  and  $u_{10}$  and  $u_{14}$  are connected by a path  $u_{10}wu_{14}$  of length 2. Now  $G$  has a 4-edge-cut  $E_1 = \{t_1, t_2, t_3, t_4\}$  as shown in Fig. 10. In an inductive way we have that  $G$  has infinite many vertices, a contradiction. If  $h_1 = h_2$  or  $h_3 = h_4$ , then  $u_{10}u_{13}$  and  $w_7w_4$  are edges of  $G$  and  $G$  has a 4-edge-cut  $E_2 = \{s_1, s_2, s_3, s_4\}$  as shown in Fig. 10. So  $G$  either has subgraph  $T$  or has infinite many vertices, a contradiction.

We show four cases of  $e_3$  as follows, the other four cases could be proved similarly. For  $e_3 = u_1u_{11}$ , we can easily obtain that  $G - S$  has more than one perfect matchings. For  $e_3 = u_1u_2$  as shown in Fig. 10(1),  $h_1$  and  $f_2$  are disjoint, and  $h_1$  and  $g_2$  are disjoint since  $h_1$  is different from  $h_5, f_5, h_4$  and  $h_2$ . Then  $\{e, u_1u_{11}\} \subset M$  and each face of  $G - \{v_1, v_2, u_1, u_{11}\}$  is bounded by a cycle. By Theorem 2.6  $G - S$  has at least two perfect matchings, a contradiction. For  $e_3 = u_7u_8$  as shown in Fig. 10(2),  $h_3$  is disjoint with  $g_2$  and  $f_2$  since  $h_3$  is different from  $h_5, f_5, h_4$  and  $h_2$ , and  $f_6$  and  $f_2$  are disjoint since  $f_6$  is different from  $h_4$  and  $h_2$ . So a similar contradiction occurs. For  $e_3 = u_8u_9$  as shown in Fig. 10(3), since  $h_5$  is not one of  $h_3, h_1, h_4$  and  $h_2$ ,  $h_5$  is disjoint with  $f_1$  and  $f_2$ . We also know that  $f_6$  and  $f_2$  are disjoint. So we have a similar contradiction.



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