# A Fast Algorithm for Computing Bipartite Edge Frustration of (5,6)–Fullerenes by Using Dual Graphs

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**Abstract.** Suppose G is a graph with the vertex set V(G). The smallest number of edges that need to be deleted from G to obtain a bipartite spanning subgraph is called the bipartite edge frustration of G and is denoted by φ(G). This graph invariant has important applications in computing stability of fullerenes. In this paper we use the concept of dual graph for obtaining the bipartite edge frustration of all (5,6)- fullerene graphs.

**Keywords:** *bipartite edge frustration, dual graph, (5,6)−fullerene.*

## 1. Introduction

A (k,6)−fullerene is a connected cubic plane graph, with faces having sizes k and 6. Recall that, in chemical graph theory, a fullerene graph is 3-regular and 3−connected. The only values of k for which a (k,6)−fullerene exists are 3, 4 and 5. A (5,6)−fullerene graph is a plane graph, with 12 faces being pentagons and the remaining faces are hexagons. We are interested in the fullerene graphs in which no two pentagons share an edge. They are called "isolated pentagons" (IPR) fullerenes. A (5,6)-fullerene is simply called a fullerene. They are molecules in the form of polyhedral closed cages made up entirely of n carbon atoms that are bonded in a nearly spherically symmetric configuration, [1,2]. Some properties of this important class of molecules are studied in [3–7].

The smallest number of edges that have to be deleted from a graph to obtain a bipartite spanning subgraph is called the bipartite edge frustration (or frustration index) of G and is denoted by φ(G). This topological index has important applications in computing stability of fullerenes. Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make the fullerene graph bipartite [8]. In [9], the authors reported some interested results in this direction and presented an intuitive proof for bipartite edge frustration of fullerenes and other polyhedral graphs. In [10], frustration index was computed for some classes of nanotubes. Moreover in [11], authors found this index of different graphs using a mathematical programming model and genetic algorithm. We studied the bipartite edge and vertex frustration of some classes of graphs, see [12–18] and also presented an algorithm for obtaining frustration index of (3,6)–fullerene graphs, see [19].

Fullerene graphs are not bipartite, and their bipartite edge frustration are positive integers. In the boundary of every odd face at least one edge must be removed and at most two odd faces can be destroyed by a removal of one edge. In what follows, important results regarding bipartite edge frustration of fullerenes are stated.

There are many forms of duality in graph theory. In this paper, we use the concept of dual graph to obtain the bipartite edge frustration of (5,6)-fullerene graphs. Given a connected plane graph G, we construct dual graph G* in the following stages:

- G* has a vertex in each face of G (the infinite face included).
- G* has an edge between two vertices, if in G two faces share an edge.

This procedure is illustrated in the Figure 1.

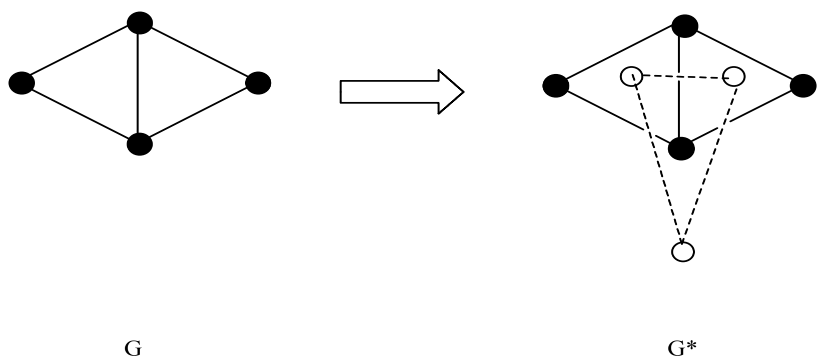


**Figure 1.** A graph G and its dual G*.

Dual graph is not always a simple graph, it might be a multigraph and a pendant edge in G gives a loop in G*. Moreover, the edge e is a loop in G if and only if e* is a bridge in G*. The number of edges forming the cycle of a face f in G is equal to the degree of the corresponding vertex f* in G*. The graph G is called self-dual, when G≈G*. A wheel graph $W_n$ is a graph with n vertices ($n \geq 3$), formed by connecting a single vertex to all vertices of a cycle of size n. Wheel graphs $W_n$ form an infinite family of self-dual graphs, see Figure 2.

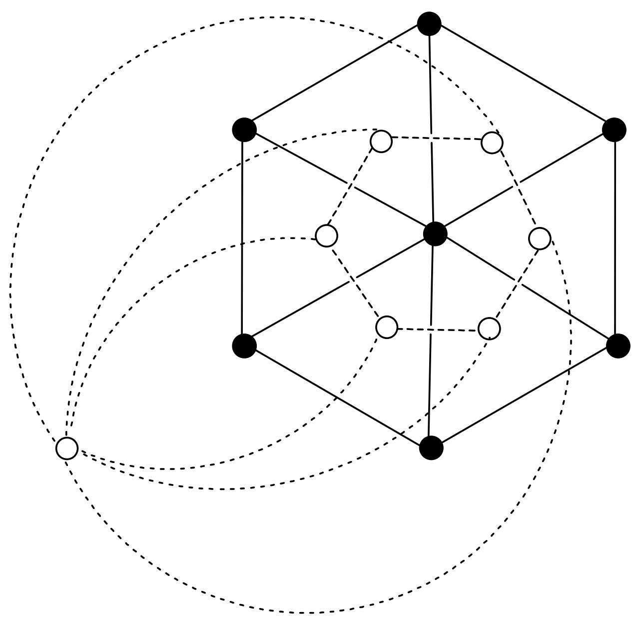

**Figure 2.** The wheel graph $W_6$ and its dual.

If G is a connected plane graph with n vertices, m edges and f faces, then G* has f vertices, m edges and n faces. Note that if G is a connected plane graph, then G* is also connected plane graph; and G is bipartite if and only if its dual graph G* is Eulerian. In this paper we use the concept of dual graph for obtaining the bipartite edge frustration of all (5,6)- fullerene graphs.

## 2. Results and discussion

The dual graph G* of a given plane graph G is a graph having a vertex for each finite internal region of G, and an edge for each edge in G joining two neighboring regions, for a certain embedding of G:

V(G*)={α | α is a finite internal region of G},

E(G*) ={αβ | α∩β={e}; e is an edge of G}.

In [9], authors presented an intuitive proof for bipartite edge frustration of fullerenes. In [14] and [17], the bipartite edge frustration of the low number of families of fullerene graphs was computed. In the following we present an algorithm to obtain the bipartite edge frustration of all (5,6) –fullerene graphs. Suppose G is a (5,6)–fullerene. In what follows, the pentagon regions of G (or corresponding vertices of G*) are denoted by $P_1$, $P_2$, $P_3$ ,..., $P_{12}$. The bipartite edge frustration, φ(G), is given by:

**Theorem**. Let G be a (5,6)–fullerene graph with the dual graph G*; then

$$\varphi(G) = \min\left\{ \sum_{\substack{i,j=1\\ i\le j}}^{12} d_{G^*}(\alpha_i,\alpha_j)) \mid \{\alpha_1,\alpha_2,\cdots,\alpha_{12}\} = \{P_1,P_2,\cdots,P_{12}\} \right\}.$$

**Proof.** Without losing of generality, we can assume that

$$\begin{aligned} l &= d_{G^*}(P_1,P_2) + d_{G^*}(P_3,P_4) + d_{G^*}(P_5,P_6) \\ &\quad + d_{G^*}(P_7,P_8) + d_{G^*}(P_9,P_{10}) + d_{G^*}(P_{11},P_{12}) \\ &= \min\{ \sum_{\substack{i,j=1\\ i\le j}}^{12} d_{G^*}(\alpha_i,\alpha_j)) \mid \{\alpha_1,\alpha_2,\cdots,\alpha_{12}\} = \{P_1,P_2,\cdots,P_{12}\}\} \end{aligned}$$

From Figure 3, one can see that by deleting $d_{G^*}(P_1,P_2)$ edges of a hexagonal chain connecting $P_1$ and $P_2$, as well as deleting $d_{G^*}(P_3,P_4)$ edges of another hexagonal chain connecting, $P_3$ and $P_4$ and by continuing this process, by deleting $d_{G^*}(P_{11},P_{12})$ edges of a hexagonal chain connecting $P_{11}$ and $P_{12}$, the resulting graph will be bipartite. Thus,

$$\begin{aligned} \varphi(G) &\le d_{G^*}(P_1,P_2) + d_{G^*}(P_3,P_4) + d_{G^*}(P_5,P_6) \\ &\quad + d_{G^*}(P_7,P_8) + d_{G^*}(P_9,P_{10}) + d_{G^*}(P_{11},P_{12}) = l. \end{aligned}$$

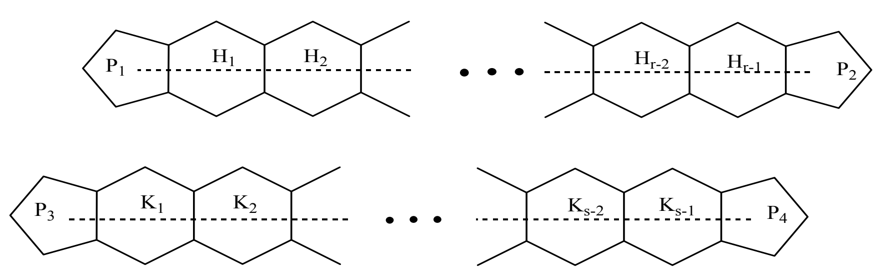


**Figure 3.** The shortest paths between pentagons.

Notice that even the hexagon chain is zig-zag, vertical edges are omitted and there is no difference in computing bipartite edge frustration of the graph.

The dual of each fullerene graph is connected, for each pentagon $P_i$ and $P_j$, $1 \le i, j \le 12$, as two vertices of dual of fullerene graph, there is a path connecting them. The end vertices of this path correspond to pentagons and other vertices correspond to hexagons.

It is sufficient to prove $\varphi(G) \ge 1$; assume first that $\varphi(G) = k$, then, by deleting k edges of G, one obtains a bipartite subgraph of G. Choose the pentagon $P_1$. By definition, there exists at least one edge $e_l$ of $P_1$ in our bipartization. Clearly, $e_l$ is a common edge of $P_1$ and one pentagon or hexagon. If $e_l$ is a common edge of $P_1$ and another pentagon then we proceed by choosing the third pentagon of G instead of $P_1$. If $e_l$ is a common edge of a pentagon and a hexagon then, by removing $e_l$, the resulting graph will have a nonagon, Figure 4.

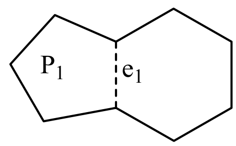


**Figure 4.** Construction of a nonagon by removing $e_l$ from G.

To find a bipartization for G, one has to remove one edge $e_2$ from this nonagon. There are two cases of deleting edge $e_2$from this nonagon: one is the common edge with a pentagon or edges from a hexagon. In the first case, we proceed choosing the third pentagon of G instead of $P_1$.In the second case, by removing $e_2$ from G, a new odd cycle will be constructed, Figure 5.

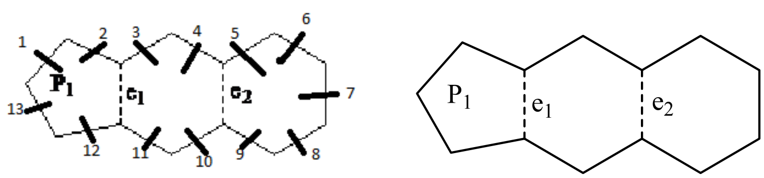


**Figure 5.** Construction of a new odd cycle by removing $e_2$ from G.

Continue this process to obtain an edge from the second pentagon of G, say $P_2$. Suppose, by removing r edges of G we achieve to $P_2$. Thus, we will find a path connecting vertices u and v in G* corresponding to pentagons $P_1$ and $P_2$ of G, Figure 6. Hence $d_{G*}(P_1, P_2) \le r$ and so by deleting r edges of G we will find an even cycle surrounding two pentagons of G. Choose the pentagon $P_3$ and continue the process. One edge $f_l$has to be deleted from $P_3$ in this bipartization. The edge $f_l$ is a common edge of two pentagons or a pentagon of an even cycle C. If $f_l$ is an edge of even cycle C then by deleting $f_l$ an odd cycle C′ will be constructed.

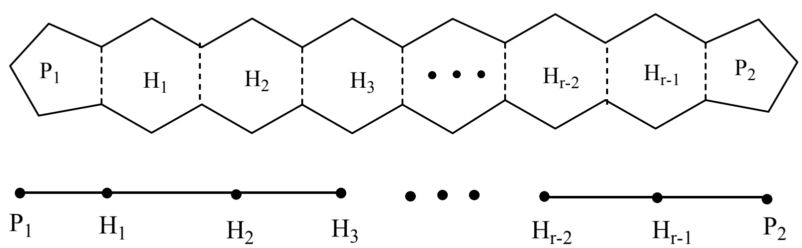


**Figure 6.** A part of (5,6)–fullerene G and its corresponding path in G*.

In this bipartization, one edge from C′ has to be deleted. Continue this process to attain $P_4$ or an even cycle C. The same process is needed for the pentagon $P_4$. Assume that the sum of the length of two shortest path between $P_1$, $P_2$ ,$P_3$ and $P_4$ is less or equal to r+s. Without loss of generality, we assume that

$$d_{G*}(P_1,P_2)+d_{G*}(P_3,P_4)\leq r+s.$$

There are various cases for the path between $P_1$ and $P_2$ and the path $P_3$ and $P_4$. These paths may be disjoint, such as in Figure 7, or may have a common vertex, as shown in Figure 8.

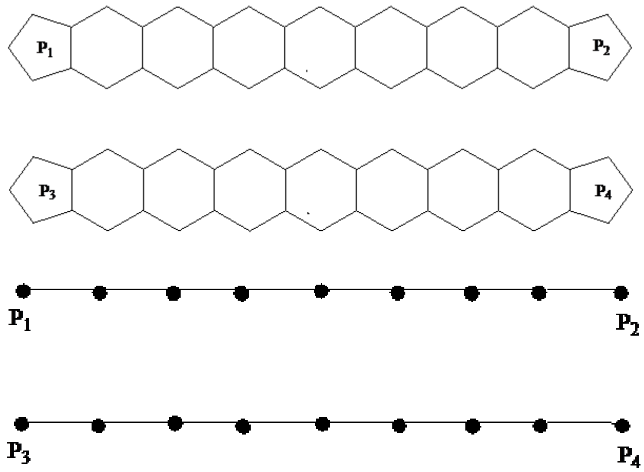


**Figure 7.** Two disjoint paths between pentagons as vertices of G*.

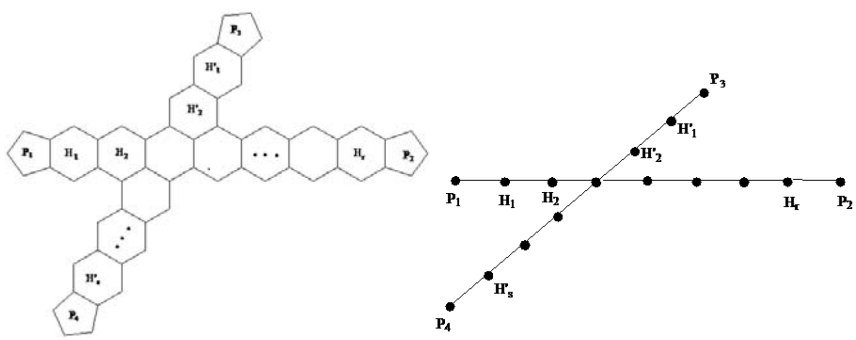


**Figure 8.** Two paths with a common vertex.

If there is more than one common vertex, (see Figure 9), one can find two shortest paths between four pentagons $P_1$, $P_2$, $P_3$ and $P_4$. For example, the sum of the lengths of path between $P_1$ and $P_3$ and path between $P_2$ and $P_4$, may be less than the sum of the lengths of path between $P_1$ and $P_2$ and path between $P_3$ and $P_4$.

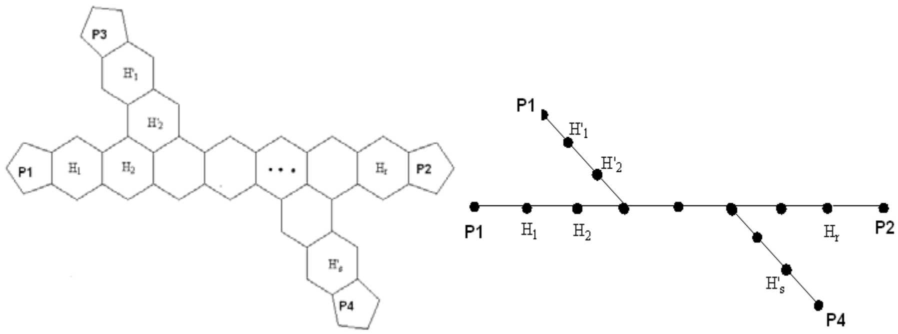


**Figure 9.** Two paths with some common vertices.

Now we choose the pentagon $P_5$ and continue the process. Suppose that the length of shortest path between $P_5$ and the remaining pentagons is t, again without reducing the generality, we can say that $dG^*(P_5, P_6) \leq t$ and then

$$d_{G^*}(P_1,P_2) + d_{G^*}(P_3,P_4) + d_{G^*}(P_5,P_6) \leq r+s+t.$$

There are various cases for the path between $P_1$ and $P_2$, the path $P_3$ and $P_4$ and the path between $P_5$ and $P_6$:

**Case 1**. All paths are disjoint.

**Case 2**. The third path has a common vertex with first path and a common vertex with second path, see Figure 10.

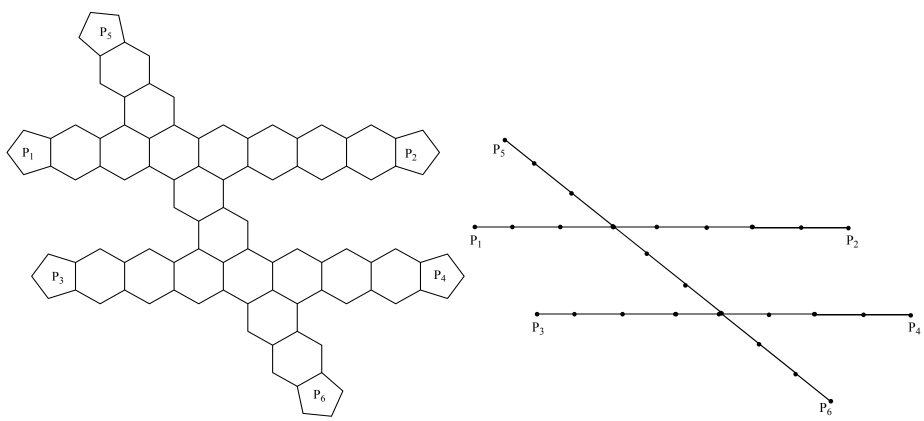


**Figure 10.** The third path has a common vertex with each another paths.

**Case 3**. The third path has a common vertex with just one of the first and second path, such as in Figure 11.

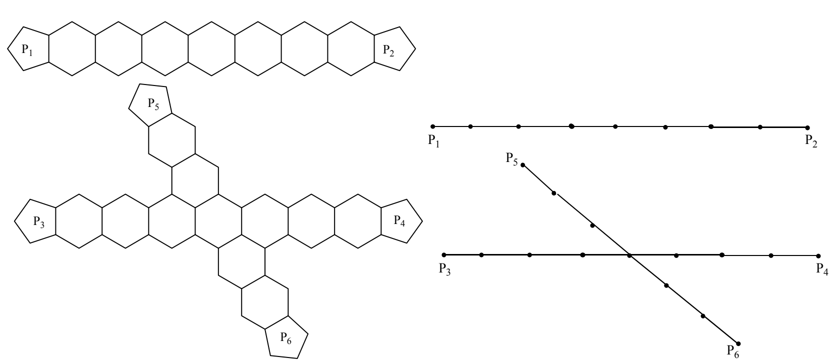

**Figure 11.** The third path has a common vertex with one of another paths.

**Case 4**. All three paths have a common vertex, Figure 12.

We must assume that, the case in Figure 13, doesn't happen, because, one can find three shortest paths between pentagons $P_1$, $P_2$, $P_3$, $P_4$, $P_5$ and $P_6$, which minimum value of the sum of lengths can be achieved for less than the previous value. For the example in Figure 13, we have:

$$d_{G^*}(P_1,P_3)+d_{G^*}(P_4,P_5)+d_{G^*}(P_2,P_6)\le d_{G^*}(P_1,P_2)+d_{G^*}(P_3,P_4)+d_{G^*}(P_5,P_6)$$

By continuing this process, in this step we choose $P_7$. Suppose that the length of shortest path between $P_7$ and remaining pentagons is x, again without reducing the generality, we can say that $d_{G^*}(P_7, P_8) \le x$ and then

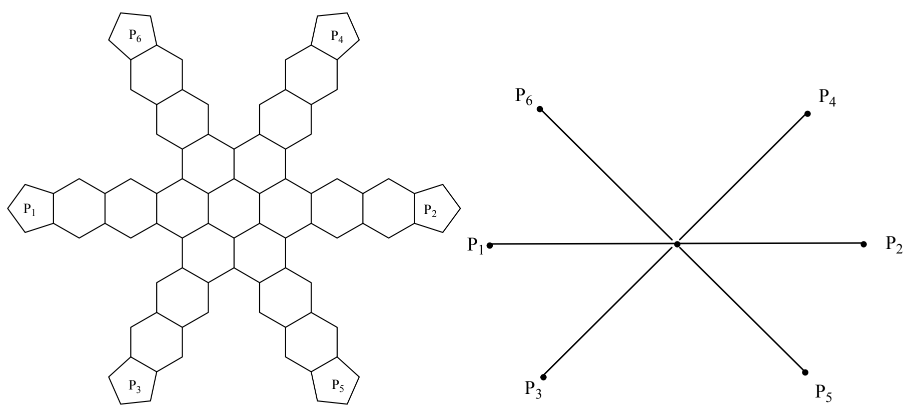


**Figure 12.** Three paths are common in one vertex.

$$d_{G^*}(P_1,P_2)+d_{G^*}(P_3,P_4)+d_{G^*}(P_5,P_6)+d_{G^*}(P_7,P_8)\le r+s+t+x.$$

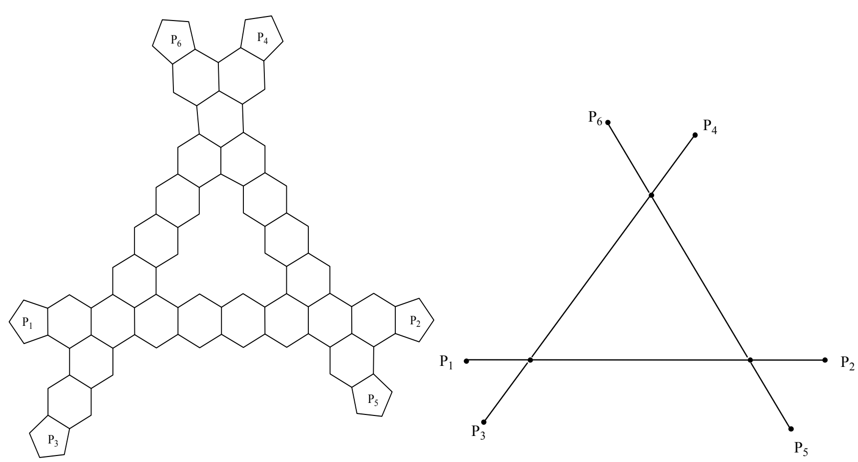


**Figure 13.** A case that doesn't happen.

By the above argument one can see that there are various cases for the path between $P_1$ and $P_2$, the path $P_3$ and $P_4$, and so one. We must to assume that the case in Figure 14 (a), doesn't happen. Because, we can find three shortest paths between pentagons $P_1$, $P_2$, $P_3$, $P_4$, $P_5$, $P_6$, $P_7$ and $P_8$ which minimum value of the sum of lengths can be achieved for less than the previous value. Moreover, the case in Figure 15, doesn't happen, because a hexagon could be common at most three chains of hexagon, see Figure 14.

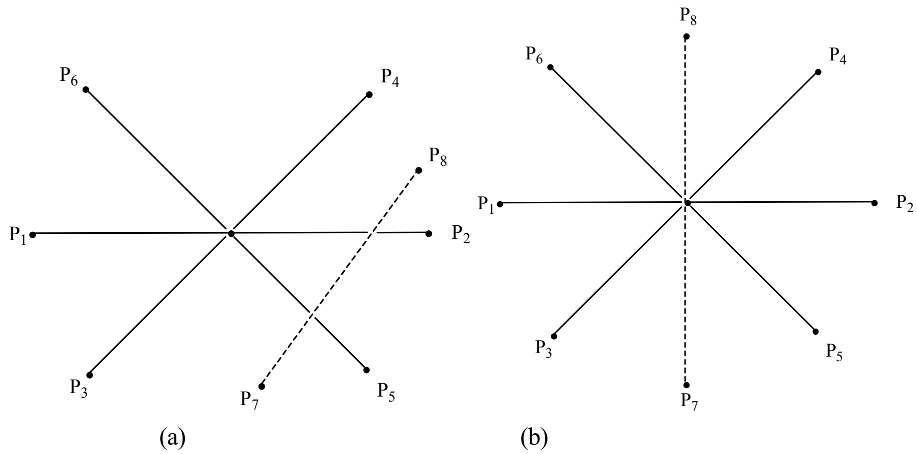


**Figure 14.** Cases that do not happen.

By continuing this process, in the following steps, we choose $P_9$ and by deleting an edge one achieves $P_{10}$ and vice-versa and finally choose $P_{11}$ and achieve $P_{12}$ and vice-versa. Then $d_{G^*}(P_9, P_{10}) \leq y$ and $d_{G^*}(P_{11}, P_{12}) \leq z$ and

$$d_{G^*}(P_1,P_2)+d_{G^*}(P_3,P_4)+d_{G^*}(P_5,P_6) \\ +d_{G^*}(P_7,P_8)+d_{G^*}(P_9,P_{10})+d_{G^*}(P_{11},P_{12})\leq r+s+t+x+y+z$$

Our main proof will consider the following argument. In the process of deleting edges, for destroying two final pentagons (without loss of generality) we achieve $P_{12}$ from $P_{11}$ or vice-versa. In this case, we just delete edges from the hexagons not any even cycle C. If z is the number of deleted edges then z will be different from r+s+t+x+y edges removed before. Thus,

$$\begin{aligned}\phi(G)&=k=r+s+t+x+y+z\\ &\geq d_{G^*}(P_1,P_2)+d_{G^*}(P_3,P_4)+d_{G^*}(P_5,P_6)\\ &+d_{G^*}(P_7,P_8)+d_{G^*}(P_9,P_{10})+d_{G^*}(P_{11},P_{12})\\ &\geq \min\{\sum_{\substack{i,j=1\\ i\leq j}}^{12} d_{G^*}(\alpha_i,\alpha_j))\mid\{\alpha_1,\alpha_2,\cdots,\alpha_{12}\}=\{P_1,P_2,\cdots,P_{12}\}\}.\end{aligned}$$

In the process of deleting edges, we achieve even cycles C (different of a hexagon) from $P_{11}$ and $P_{12}$. Suppose $g_1$ and $g_2$ are the first deleted edges of even cycle C in this process. If there exists one common edge in the process of achieving $P_{11}$ from $P_{12}$ and vice-versa then $d_{G^*}(P_{11}, P_{12}) \leq z$ and a similar argument as above is used. If in the process of achieving $P_{11}$ from $P_{12}$ and vice-versa there is no common edge and between edges $g_1$ and $g_2$ the edge $g_2$ is closer to $P_{12}$ then

$$\begin{aligned}\phi(G) &= k = r+s+t+x+y+z \\ &\geq d_{G^*}(P_1,P_2)+d_{G^*}(P_3,P_4)+d_{G^*}(P_5,P_6) \\ &+d_{G^*}(P_7,P_8)+d_{G^*}(P_9,P_{10})+d_{G^*}(P_{11},P_{12}) \\ &\geq \min\{\sum_{\substack{i,j=1 \\ i\leq j}}^{12} d_{G^*}(\alpha_i,\alpha_j)) \mid \{\alpha_1,\alpha_2,\cdots,\alpha_{12}\}=\{P_1,P_2,\cdots,P_{12}\}\}.\end{aligned}$$

which completes our argument.

Finally, in the following example, we apply our main result to compute the edge frustration index of an infinite family of (5,6)-fullerene graphs.

**Example.** Let $C_{40n+6}$ be the (5,6)-fullerene graph with 40n+6 vertices depicted in Figure 15. To obtain a bipartite subgraph of $C_{40n+6}$, we must obtain bipartite subgraphs with destroying all pentagons.

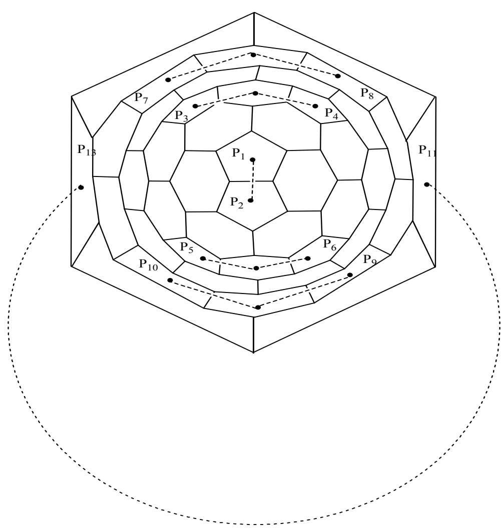


**Figure 15.** Shortest path between pentagons as vertices of $C^*_{40n+6}$.

It is easy to see that

$$\begin{aligned}&\min\{\ d_{G^*}(P_1,P_i) \mid 2\leq i\leq 12\} = \min\{\ d_{G^*}(P_2,P_i) \mid 1\leq i\leq 12, i\neq 2\} = d_{G^*}(P_1,P_2)=1 \\ &\min\{\ d_{G^*}(P_3,P_i) \mid 1\leq i\leq 12, i\neq 3\} = \min\{\ d_{G^*}(P_4,P_i) \mid 1\leq i\leq 12, i\neq 4\} = d_{G^*}(P_3,P_4)=2 \\ &\min\{\ d_{G^*}(P_5,P_i) \mid 1\leq i\leq 12, i\neq 5\} = \min\{\ d_{G^*}(P_6,P_i) \mid 1\leq i\leq 12, i\neq 6\} = d_{G^*}(P_5,P_6)=2 \\ &\min\{\ d_{G^*}(P_7,P_i) \mid 1\leq i\leq 12, i\neq 7\} = \min\{\ d_{G^*}(P_8,P_i) \mid 1\leq i\leq 12, i\neq 8\} = d_{G^*}(P_7,P_8)=2 \\ &\min\{\ d_{G^*}(P_9,P_i) \mid 1\leq i\leq 12, i\neq 9\} = \min\{\ d_{G^*}(P_{10},P_i) \mid 1\leq i\leq 12, i\neq 10\} = d_{G^*}(P_9,P_{10})=2 \\ &\min\{\ d_{G^*}(P_{11},P_i) \mid 1\leq i\leq 12, i\neq 11\} = \min\{\ d_{G^*}(P_{12},P_i) \mid 1\leq i\leq 12, i\neq 12\} = d_{G^*}(P_{11},P_{12})=2\end{aligned}$$

Then, we apply our main theorem to prove that

$$\varphi(C_{40n+6}) = \min\left\{\sum_{\substack{i,j=1\\ i\le j}}^{12} d_{G*}(\alpha_i,\alpha_j)) \mid \{\alpha_1,\alpha_2,\cdots,\alpha_{12}\} = \{P_1,P_2,\cdots,P_{12}\}\right\}$$

$$= \{d_{G^*}(P_1,P_2) + d_{G^*}(P_3,P_4) + d_{G^*}(P_5,P_6) + d_{G^*}(P_7,P_8)$$

$$+ d_{G^*}(P_9,P_{10}) + d_{G^*}(P_{11},P_{12})\}$$

$$= 1+2+2+2+2+2$$

$$= 11.$$

By the above argument we can obtain the bipartite edge frustration of all families of (5,6)-fullerene graphs.

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