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Research Paper

On the Number of Perfect Star Packing and Perfect Pseudo-Matching in Some Fullerene Graphs

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Abstract

A perfect star packing in a fullerene graph G is a spanning subgraph of G whose every component is isomorphic to the star graph $K_{1,3}$. A perfect pseudo-matching of a fullerene graph G is a spanning subgraph H of G such that each component of H is either K_2 or $K_{1,3}$. In this paper, we calculate the number of perfect star packing in some $(3,6)$-fullerene graphs and perfect pseudo-matching in Chamfered fullerene graphs.

1 Introduction

Fullerenes are polyhedral molecules containing only carbon atoms and pentagonal and hexagonal faces. The first fullerene molecule was discovered experimentally in 1985 by Kroto et al. [1]. The discovered molecule, C_{60}, comprises only 60 carbon atoms and resembles Buckminster Fuller's geodesic dome. Thus, it was named buckminsterfullerene. Fullerene graphs are 3-regular, 3-connected, planar graphs with pentagonal and hexagonal faces. Euler's formula follows that every fullerene graph's number of pentagonal faces is always twelve. The existence of such graphs on n vertices was established for all even $n \geq 20$ except $n = 22$ in a paper by Grunbaum and Motzkin [2]. Klien and Liu [3] show that fullerene graphs exist on n vertices with isolated pentagons for $n=60$ and for each even $n \geq 70$. To study some introductions on fullerene graphs, we refer the reader to [4, 5]. Also, there are two infinite classes of fullerene graphs, the ones with pentagons replaced by triangles and the ones with pentagons replaced by squares. They are known as $(3,6)-$fullerenes and $(4,6)-$fullerenes, respectively.

A matching in a graph G is a set of independent edges of G, i.e., a set of edges such that no two edges share a vertex. A matching is said to be perfect if every vertex of G is incident with an edge from it. In chemistry, the perfect matching is called **Kekulé structures**. In other

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words, a perfect matching is a spanning subgraph whose all components are isomorphic to K_2. All fullerene graphs have perfect matchings since they have no bridges [6].

For given graphs, G and H, a perfect H-packing in G is a spanning subgraph of G whose all components are isomorphic to H. If H is the star graph $K_{1,3}$, it is called perfect star packing. We refer the reader to [7, 8] for recent results and developments in this subject. In [9], authors investigated which fullerene graphs allowed perfect star packings and defined a type of perfect star packing called $P0$. A perfect star packing in G is of type $P0$ if no center of a star lies on a pentagon of G. If in a spanning subgraph of G, each component is isomorphic to $K_{1,3}$ or to K_2, then we have perfect pseudo-matching. For more on the problem of pseudo-matching and the size of a perfect pseudo-matching in fullerene graphs, see [10].

In the two following sections, we investigate the number of perfect star packings and perfect pseudo-matching in some fullerene graphs. Section 4 presents two forbidden configurations whose presence in a fullerene graph G precludes the existence of a perfect star packing.

2 Number of perfect star packing in $(3,6)$-fullerene graphs

In the following, for a fullerene graph G, we denote by $PSP(G)$ the number of perfect star packing in G. In each perfect star packing in a $(3,6)$-fullerene graph, each triangle has a maximum of one central vertex of the star. So, the packing of each triangle can be in the following two forms. (Figure 1.)

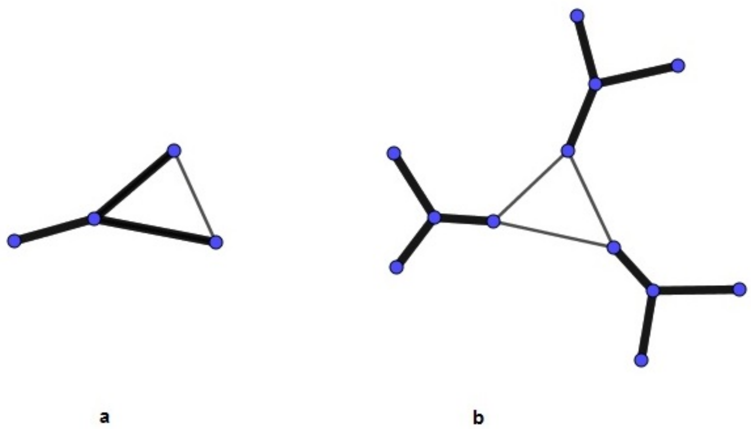

Figure 1: Possible modes of packing a triangle.

Based on this, we examine the star packing in $(3,6)$-fullerene graphs in different cases. We have found in [9] a method for perfect star packing in $(3,6)$-fullerene graphs. $(3,6)$-fullerenes with isolate triangles are called non-trivial and $(3,6)$-fullerenes with a pair of adjacent triangles are known as trivial. Trivial $(3,6)$-fullerene graphs consisting of r concentric layers of hexagons and two caps formed by two adjacent triangles. In the rest of this section, we will restrict to trivial $(3,6)$-fullerene graphs.

This section examines the different states of perfect star packing in trivial $(3,6)$-fullerene graphs. In paper [9], a perfect star packing for fullerene graphs is presented. Accordingly, we will investigate how many possible packings are for trivial $(3,6)$-fullerene graphs. A $(3,6)$-fullerene is defined by a triple (r,s,t) of non-negative integers, where r represents the number of hexagonal layers, s represents the number of spokes within each layer, and t represents the twist. If G is a non-trivial $(3, 6)$-fullerene graph, s is at least 2.

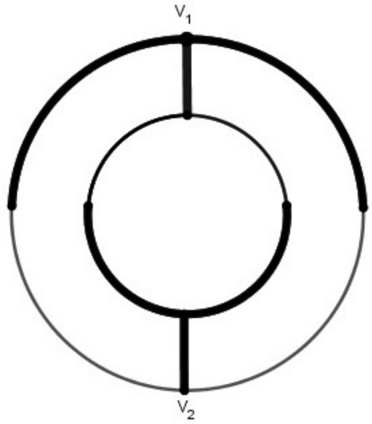

Figure 2: Star packing in two circles.

First, we consider a packing of two circles in $(3, 6)$-fullerene graphs, as shown in Figure 2. In this packing, vertex v_1 is the center of a star. Next, we will have another packing in these two circles by rotating the outer circle and considering vertex v_2 as the center of a star. If r is even, we can cover vertices in all rings with this packing. If r is odd, we continue the above process for the number of $r-1$ circles; that is, we put a star in each pair of circles. Finally, one circle remains, which is the cap. According to the issues raised in Theorem 25 of [9], there are two packages for the cap. An example of packing in a $(3, 6)$-fullerene graph is shown in Figure 3. In Figure 3, the vertex v_1 is a central vertex of a star. If v_3 is in the center of one star, we see the situation in Figure 4.

So, the two inner circles can also have two packing modes. (v_1 or v_3 are in the center of stars) Thus we can consider many packings for a trivial $(3, 6)$-fullerene graph. According to the above argument, we will have the following theorem for trivial $(3, 6)$-Fullerene graphs.

Theorem 2.1. *Let G be a trivial $(3, 6)$-Fullerene graph. Then $PSP(G) = 3(2^{\frac{r}{2}})$ if r is even, and $PSP(G) = 2^{\frac{r+3}{2}}$ if r is odd.*

Proof. In trivial cases, we consider four cases to cover caps as shown in Figure 5. We first consider the case **a**. Then, to cover vertex V_1, vertex V_2 must be the central vertex of the star. (See Figure 6).

So, we have covered the two inner circles in one mode. Now we consider each pair of consecutive circles. We place the stars alternately on the inner and outer remaining circles, resulting in a star packing for G. Now consider two successive circles. We specify an arbitrary packing according to the mentioned method on these two circles (Figure 7). If r is even, we cover each pair of other circles similarly. With this, we have covered $r-2$ circles. In this packing, vertex v_1 is the center of the star. We will have another packing in these two circles by rotating in the outer circle and considering vertex v_2 as the center of a star. Therefore, except for the two inner circles that are covered in the manner shown in Figure 6, if we have r rings, then $PSP(G)$ in case **a** is equal to $2^{\frac{r-2}{2}}$. If we repeat the same process for case **d**, we will have $2^{\frac{r-2}{2}}$ more packings. Now we consider modes **b** and **c**. In the case of **b**, suppose v_2 is the center of the star. (Figure 8). To cover vertex w, one of the vertices w_1 or w_2 must be the central vertex. On the other hand, if w_1 is a central vertex, the vertex w_3 must be the central vertex, and if w_2

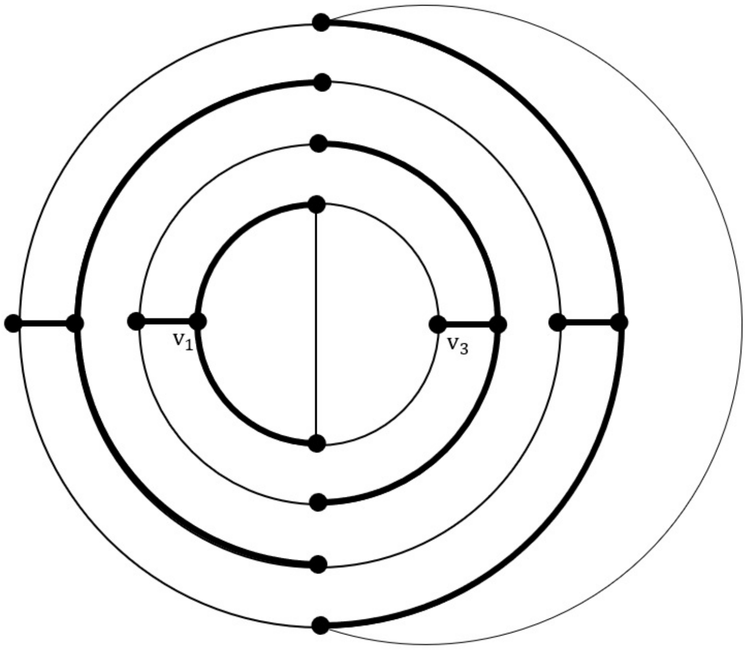

Figure 3: Perfect star packing in a trivial in a $(3, 6)$-fullerene graph.

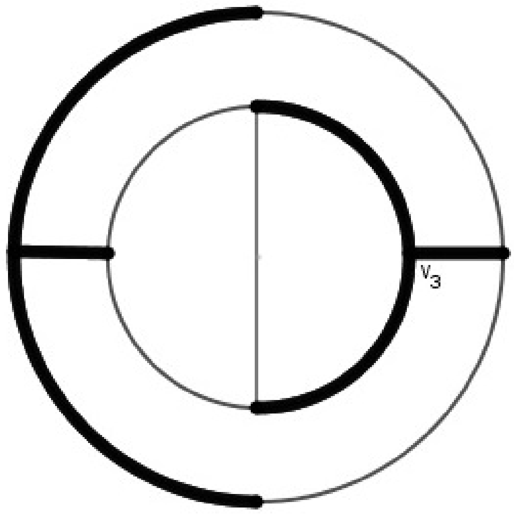

Figure 4: Vertex v_3 is in the center of one star.

is a central vertex, the vertex w_4 must also be the central vertex. So we have covered the second and third circles in two ways. If r is even, we cover each pair of other circles as mentioned in the previous case. The outermost circle, which includes the cap, can also be covered in two ways. Therefore, if we have r rings, then $PSP(G)$ in case **b** equals to $2(2^{\frac{r-2}{2}})$. If we repeat the same process for case **c**, we will have $2(2^{\frac{r-2}{2}})$packings. According to the above discussion, in the case where r is even, we have

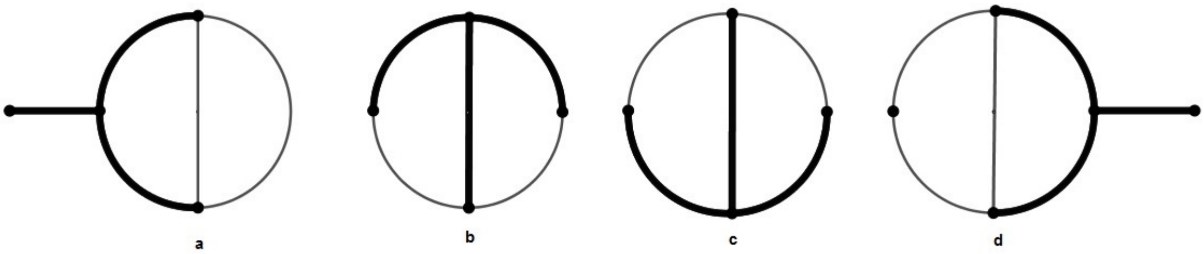

Figure 5: Four cases to cover caps.

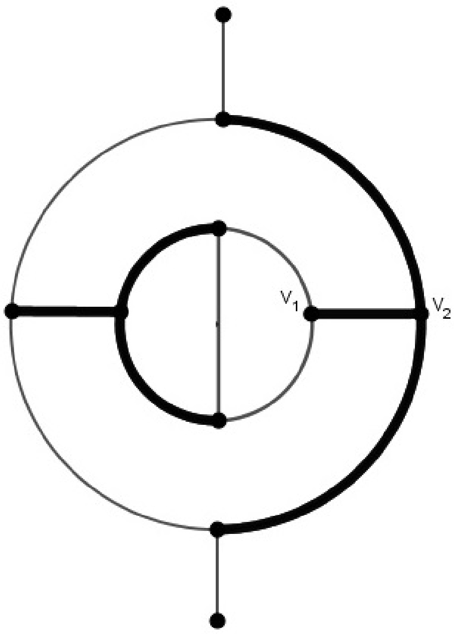

Figure 6: Case a.

$$PSP\,(G) = 2^{\frac{r-2}{2}} + 2^{\frac{r-2}{2}} + 2(2^{\frac{r-2}{2}}) + 2(2^{\frac{r-2}{2}}) = 3(2^{\frac{r}{2}}).$$

If r is odd, then with the arguments of the case that r is even, in cases **a** and **d**, we cover the two inner circles as shown in Figure 6. There are $2^{\frac{r-3}{2}}$ ways to cover the $r-3$ more circles except for the cap. Finally, we can cover the cap with 2 modes. So, in these two cases we have $2(2^{\frac{r-3}{2}})$ ways. In cases **b** and **c**, there are $2^{\frac{r-1}{2}}$ ways to cover the $r-1$ more circles. Thus in the case where r is odd, we have

$$PSP\,(G) = 2(2^{\frac{r-3}{2}}) + 2(2^{\frac{r-3}{2}}) + 2^{\frac{r-1}{2}} + 2^{\frac{r-1}{2}} = 4(2^{\frac{r-3}{2}}) + 2(2^{\frac{r-1}{2}}) = 2^{\frac{r+3}{2}}.$$

∎

For example, all possible modes in the case $r = 2$ are shown in Figure 9.

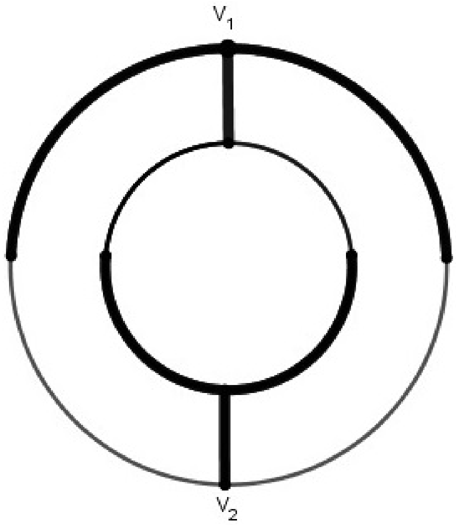

Figure 7: Star packing in two circles.

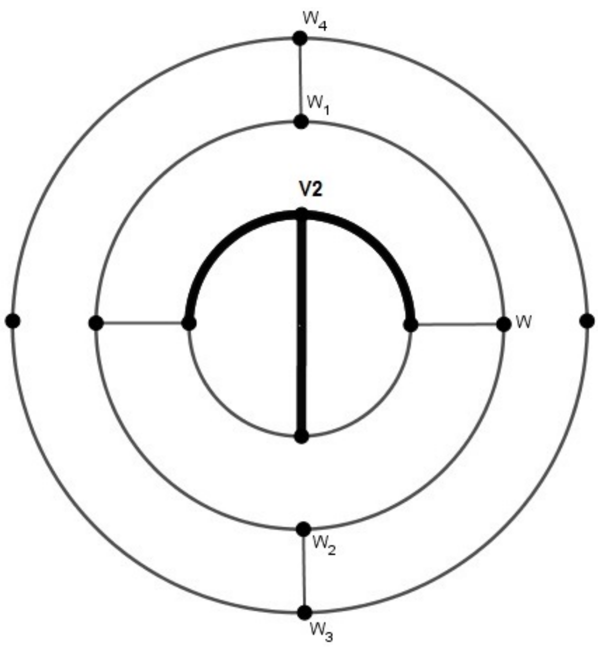

Figure 8: Vertex v_2 is in the center of one star.

3 Number of perfect pseudo-matching in chamfered fullerene graphs

By applying some transformations, we can obtain fullerene graphs with more vertices from fullerene graphs. The number of vertices in the resulting graph is usually a multiple of the number of vertices in the original graph. One of these transformations is the leapfrog transfor-

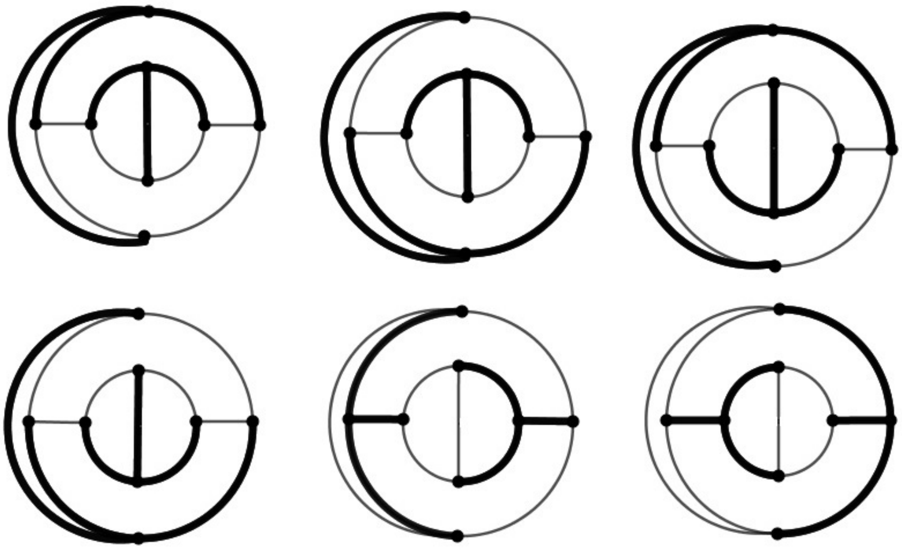

Figure 9: All modes of perfect star packing in case $r = 2$.

mation, which can be considered a truncation of the dual. It is seen that this operation triples the number of vertices. Two other examples of these transformations are Chamfer and Capra. We refer the reader to [11–14] for more information on these and some other transformations.

In this section, we will continue our discussion on how to work with Chamfer transformation. Let G is a Fullerene graph. First, we draw a similar face in each face of G, as shown in Figure 10. By connecting each vertex of the original fullerene to three vertices new polygon vertices, (Thick lines in Figure 10) we complete the next step. Finally, erase the edges of the starting fullerene. The resulting graph contains precisely twelve pentagons. The number of vertices in the new fullerene is four times the number in the original fullerene. As the resulting graph is clearly planar, 3-regular, and 3-connected, it is a fullerene graph. The resulting fullerene is called Chamfered fullerene. The readers can see [15, 16] for more on the problem of Chamfered and leapfrog fullerene graphs.

Theorem 3.1. *For all $n \geq 80$, there are Chamfered fullerene graphs containing a mixed perfect pseudo-matching with $\frac{n}{4}$ stars and t disjoint copies of K_2 components. Where $t \in \mathbb{N}$, $1 \leq t \leq 6$.*

Proof. As we know, we obtain a fullerene graph with $4k$ vertices by applying a Chamfer transformation on each k vertices of the fullerene graph. The smallest Chamfer fullerene graph has 80 vertices. It is icosahedral C_{80} isomer that arises from the unique C_{20} isomer by the Chamfer quadrupling transformation. For all $n \geq 80$, every Chamfer fullerene graphs have a perfect star packing of type $P0$. [9]. (See Figure 11). Suppose P_1 and P_2 are the two pentagons in Figure 12 that are adjacent to the original fullerene graph.

By performing Endo-Kroto 2 vertex insertion, we obtain a fullerene graph on $8m+2$ vertices with one K_2 component and $\frac{n}{4}$ stars. Furthermore, we will get a verdict if we repeat this operation for any pair of pentagons with a common edge in the original fullerene graph. ■

Figure 13 shows a perfect pseudo-matching in $C_{80}(I_h)$ with six K_2 components.

Theorem 3.2. *Let G be a Chamfered fullerene graph on n vertices; then G has a mixed perfect pseudo-matching with $\frac{n-4k}{4}$ stars and $2k$, K_2 components.*

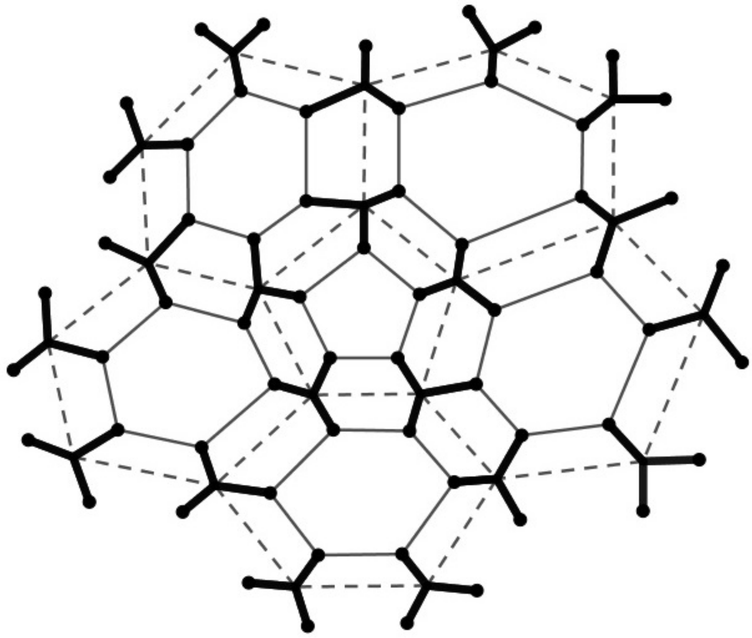

Figure 10: Chamfer transformation.

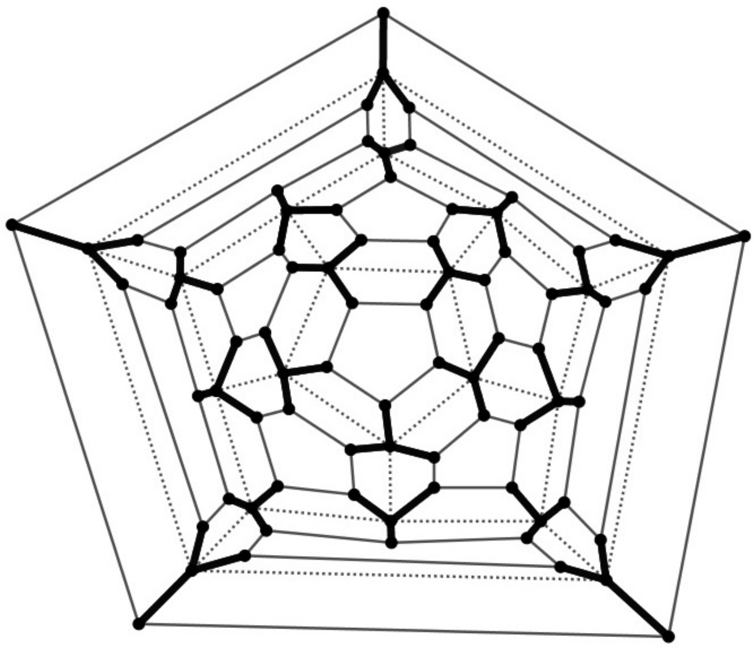

Figure 11: Perfect star packing of type $P0$.

Proof. From [9], every Chamfered fullerene graph like G has a perfect star packing of type $P0$. (That no center of a star is on a pentagon of G, and all center of stars is on hexagons). Thus,

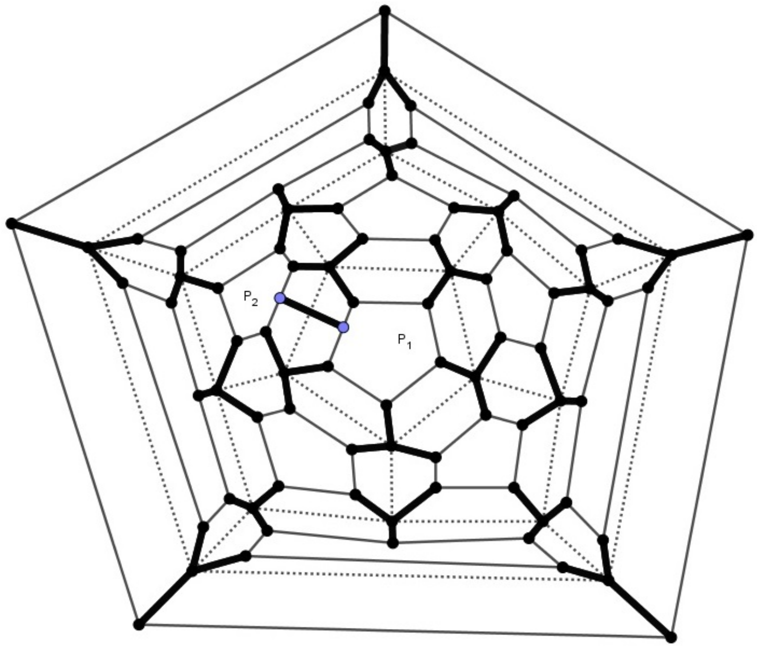

Figure 12: Pentagons P_1, P_2.

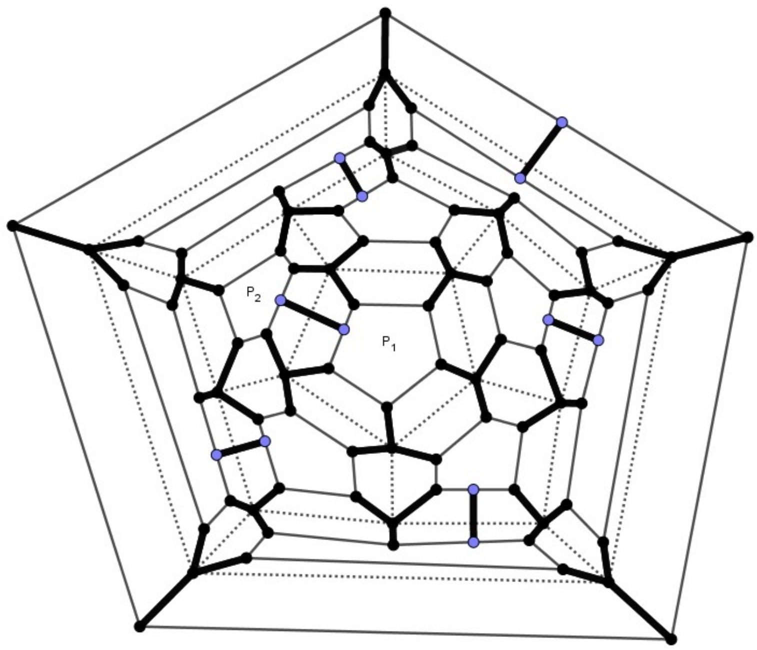

Figure 13: Perfect pseudo-matching in $C_{80}(I_h)$.

we will have packing in each hexagon, as shown in Figure 14.

The number of stars in this packing is equal to $\frac{n}{4}$. If we change the packing on a hexagon H,

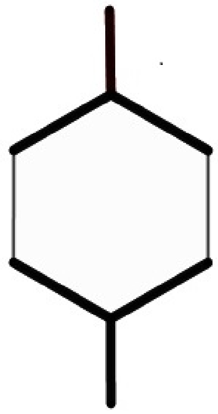

Figure 14: A packing in a hexagon.

as shown in Figure 15, we will have a packing with $\frac{n}{4}-2=\frac{n-8}{4}$ stars and four K_2 components. We get the desired by continuing this process for all G hexagons. ■

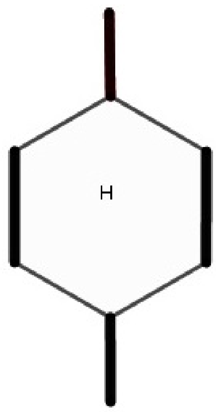

Figure 15: A packing in hexagon H.

4 Fullerene graphs with *psp* equal to zero

From [9], we know that a fullerene graph G with some forbidden configurations cannot have a perfect star packing of type $P0$. Now we list two other forbidden configurations. Therefore if these forbidden configurations exist in a fullerene graph G, then G does not have a perfect star packing of type $P0$.

Proposition 4.1. *If a fullerene graph G contains a subgraph, as shown in Figure 15, it cannot have a perfect star packing of type $P0$.*

Proof. We suppose G has a perfect star packing of type $P0$. Then, if part b in Figure 16 is a subgraph of G (For the other case, we can Let's conclude with a similar discussion), for cover

v_1, the vertex u_1 must be the center of a star because, in a perfect star packing of type $P0$, no center of a star is on a pentagon of G. On the other hand, to cover v_2, the vertex u_2 must be the star's center, which is impossible. ■

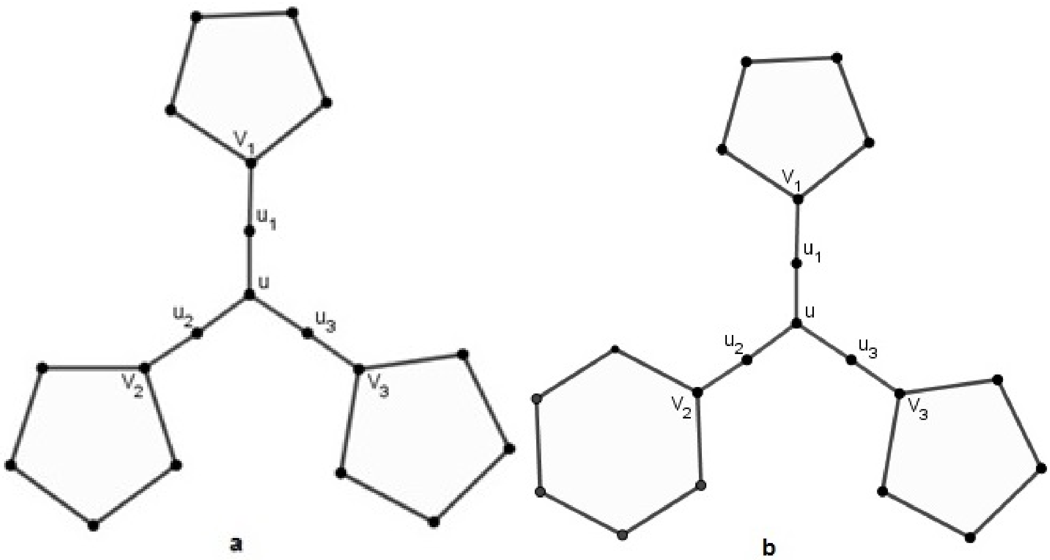

Figure 16: Two forbidden configurations.

Let us denote by $PSP0(G)$ the number of perfect star packing of type $P0$; then, we will have the following corollary.

Corollary 4.2. *Let G be a fullerene graph containing the forbidden subgraphs of Proposition 4.1, then $PSP0(G) = 0$.*

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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