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New Expansion for Certain Isomers of Various Classes of Fullerenes

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Abstract

This paper is dedicated to propose an algorithm in order to generate the certain isomers of some well-known fullerene bases. Furthermore, we enlist the bipartite edge frustration correlated with some of symmetrically distinct infinite families of fullerenes generated by the offered process.

Keywords: Fullerene, edge frustration, planar graph.

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1. Introduction

Fullerene graphs are mathematical patterns of fullerene molecules, i.e., molecules made up only by carbon atoms different than graphites and diamonds which has received the major attention in the scientific literature. For instance, Alizadeh et al. [1] investigated on some properties of nanotubical fullerenes, Andova et al. [2–4] studied on some related invariants of fullerene graphs using the terms of diameter and saturation number in graph, Brinkmann et al. presented a fast and complete method to enumerate fullerene structures in [5] and described an efficient new algorithm for the generation of fullerenes in [6]. Došlić et al. [7–10] has focused on the fullerene structures and obtained some results related with spectral properties together with computing the so-called bipartite edge frustration in such graphs. Fowler et al. have various investigations on fullerene structures which were inspiring for researchers and initiated several papers in this field of graph theory. They presented some results on independence number and fullerene stability in [12], studied all possible symmetries of fullerene structures in [13] and a special fullerene cage, so-called geometrical "leapfrog" transformation in [14].

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Recently, Hua et al. [15] considered a certain class of fullerenes with exactly $12n$ carbon atoms and studied on their Wiener and Wiener polarity indices.

We know that in graph theoretical terms, fullerene graphs with size n belong to the class of cubic, 3-connected, planar graphs with exactly 12 pentagonal faces, while all other faces are hexagons with the number $F_6 := \frac{n}{2} - 10$ using the Euler's polyhedron formula and the property of 3-regularity. It means that we can suggest the notational formula C_{20+2F_6} ($F_6 \geq 0$ and $F_6 \neq 1$) for carbon fullerenes. The smallest possible fullerene is C_{20} ($F_6 = 0$) which is an unsaturated version of dodecahedrane (known as a chemical compound) and is a dodecahedron comprised with 12 connected pentagons, and the only Platonic solid in the family of fullerene polyhedra.

The problem of enlisting all fullerene isomers with a given number of carbon atoms has drawn a remarkable amount of attention. The first tool was the spiral algorithm [16], which was demonstrated to be incomplete in that some isomers are eliminated [17].

The focus of our research is to propose a novel approach to generate some infinite classes of non-IP (without isolated pentagon) fullerenes based on a series of small fullerenes which are symmetrically different in order to predict and study the structure of high-order fullerenes in further investigations. We also remark that this method can also be efficient for IP fullerenes.

2. Construction of Fullerene Graphs with New Expansion

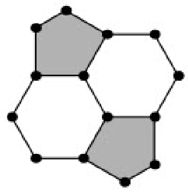
As starting point, let us to consider, for instance, C_{20} (the dodecahedron) as the smallest fullerene. In the following we define a new expansion to generate an isomer of fullerene C_{10n} with non-IP property.

As we know from the literature, fullerenes can be created from other fullerenes with two simple techniques; rearranging the faces known as Stone-Wales rearrangement, or by adding two new vertices with Endo-Kroto insertion:

- *The Stone-Wales rearrangement* [18] is a transformation that constructs an isomer of a fullerene graph. This transformation rearranges the pentagons and hexagons in a patch with two pentagons and two hexagons without changing the number of vertices as depicted in Figure 1. We recall that a patch is a 2-connected plane graph with only pentagonal or hexagonal faces, except maybe one (the unbounded) face.

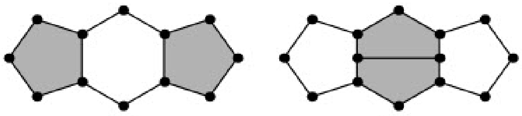
- *The Endo-Kroto C2 insertion* [11] is a transformation that results a bigger fullerene, i.e., a fullerene on $n + 2$ vertices. This transformation is possible only if the fullerene contains a patch as shown by Figure 2.

Here, we give a new method to result a bigger fullerene which can be used to almost all small fullerenes from various symmetry groups (including 28 groups).



(a) (b)

Figure 1: Stone-Wales rearrangement which replaces the patch (a) by the patch (b).



(c) (d)

Figure 2: Endo-Kroto C2 insertion which exchanges the patch (c) for the patch (d), and then inserts two new vertices.

Sun-shaped insertion: In order to do this, we insert a graph of order n, say sun-shaped graph dedicated by $Su(n)$, to a fullerene base and then construct a new bigger fullerene with extra n vertices (for example see Figure 3). We notice that the proposed expansion is not reducible, i.e., the operation inverse can not be defined but gives access to a list of isomers of fullerenes.

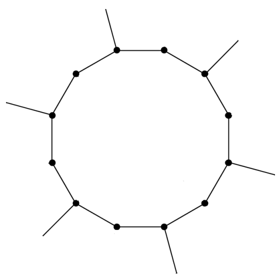


Figure 3: Sun-shaped graph $Su(12)$.

We remark that the outer edges of sun-shaped graph have been truncated, i.e., all the pendent vertices have been removed. In Figure 4, we implement this kind of insertion to C_{20} as a "seed" polyhedra.

Now, considering the sun-shaped graph (whether open or closed form), we can apply it for some classes of fullerenes with respect to the following cases:

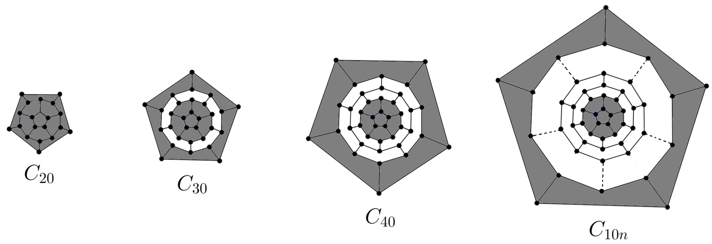


Figure 4: An isomer of fullerenes C_{10n} generated by base polyhedra C_{20} and $n-2$ sun-shaped graphs stuck together.

- **Attached hexagonal faces:** Suppose that an arbitrary fullerene has a cycle of hexagonal faces which is horizontally symmetric, i.e., these hexagonal faces are stuck together as form of (a) and not (b) in Figure 5.

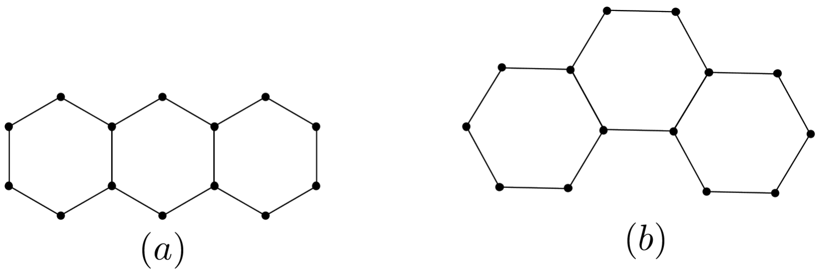


Figure 5: Permissible case (a) and impermissible case (b).

Using a path we can divide the chain of hexagon into two symmetric parts such that any included hexagon has two common vertices, say, f_i with this path. Let h_i be the upper (or lower) common vertex of hexagons in the chain and g_i be the vertex in the path located in the interior of the hexagon i. Then inserting the new edge g_ih_i and fading the edge f_ih_i implies the new subgraph which can be applied to all fullerenes including the closed chain as form of (a) in Figure 5 (see also Figure 6).

- **Attached pentagonal faces:** Now, assume that an arbitrary fullerene has a cycle of attached pentagonal faces which is horizontally divided by the process similar to the last case (see Figure 7).

- **Isolated pentagonal faces:** In this case we consider a circle of hexagons which also filled with isolated pentagonal faces (see Figure 8).

Similar to Figure 4, we enlist some small fullerenes from various symmetry groups using the method mentioned as above which are depicted in Figures 9-11.

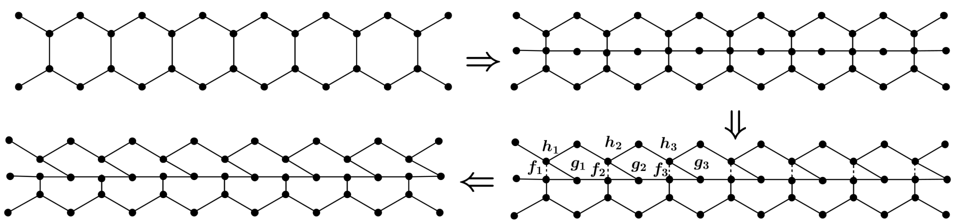


Figure 6: Illustration of the process for the case that all hexagons are stuck together.

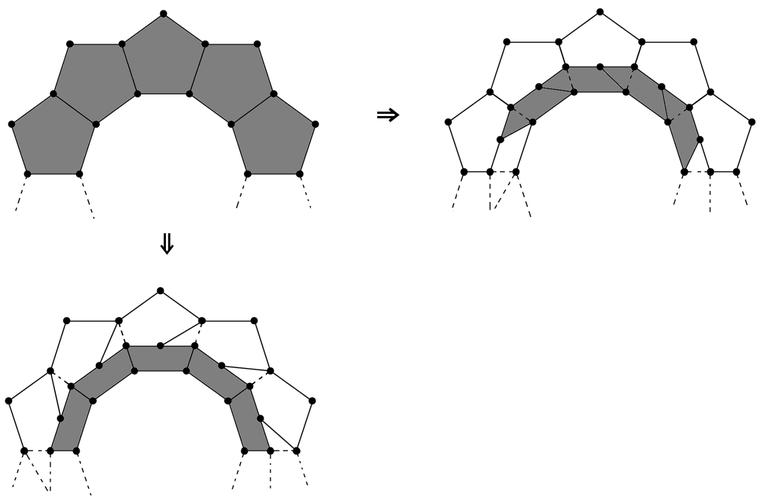


Figure 7: Illustration of the two possible processes for the case that all pentagons are stuck together.

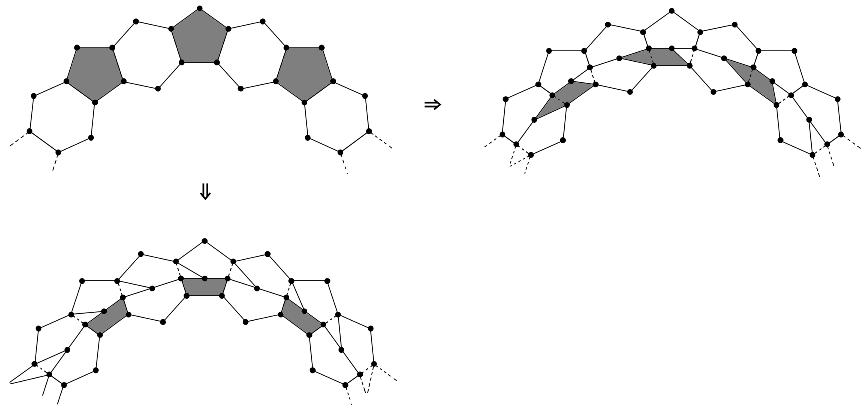


Figure 8: Illustration of the two possible processes for the case that chain contains isolated hexagons and pentagons are stuck together.

3 Edge Frustration of Fullerenes

As we know the bipartite graphs have so many novel applications and are extensively used in modeling the phenomena. Several papers have been focused on some valuable approaches to quantifying non-bipartivity of graphs. Recently, a new one has been presented which is based on counting the edges that violates the defining property of bipartite graphs. An edge $e \in E(G)$ is said to be frustrated with respect to a given bipartition (V_1, V_2) of $V(G)$ if both endpoints of e belong to the same class of the bipartition. Bipartite edge frustration of a graph G, indicated by $\varphi(G)$, is the minimum number of frustrated edges over all possible bipartitions of $V(G)$. In another word, $\varphi(G)$ is the smallest cardinality of a set of edges of G that need to be deleted to obtain a bipartite spanning subgraph.

Throughout this section, we enlist the invariant edge frustration of sun-shaped expansion (SSE) of fullerenes from some classes of symmetry groups using the sun-shaped method as mentioned in previous section.

Remark 1. *Table 1 shows that $\varphi(F_b) \leq \varphi(SSE(F_b))$ for any fullerene base F_b. This make us to conjecture that the inequality holds for the other of symmetry groups. It is also worth mentioning that here in Table 1, C_n is produced by an iteration of sun-shaped expansion method for n times, consecutively.*

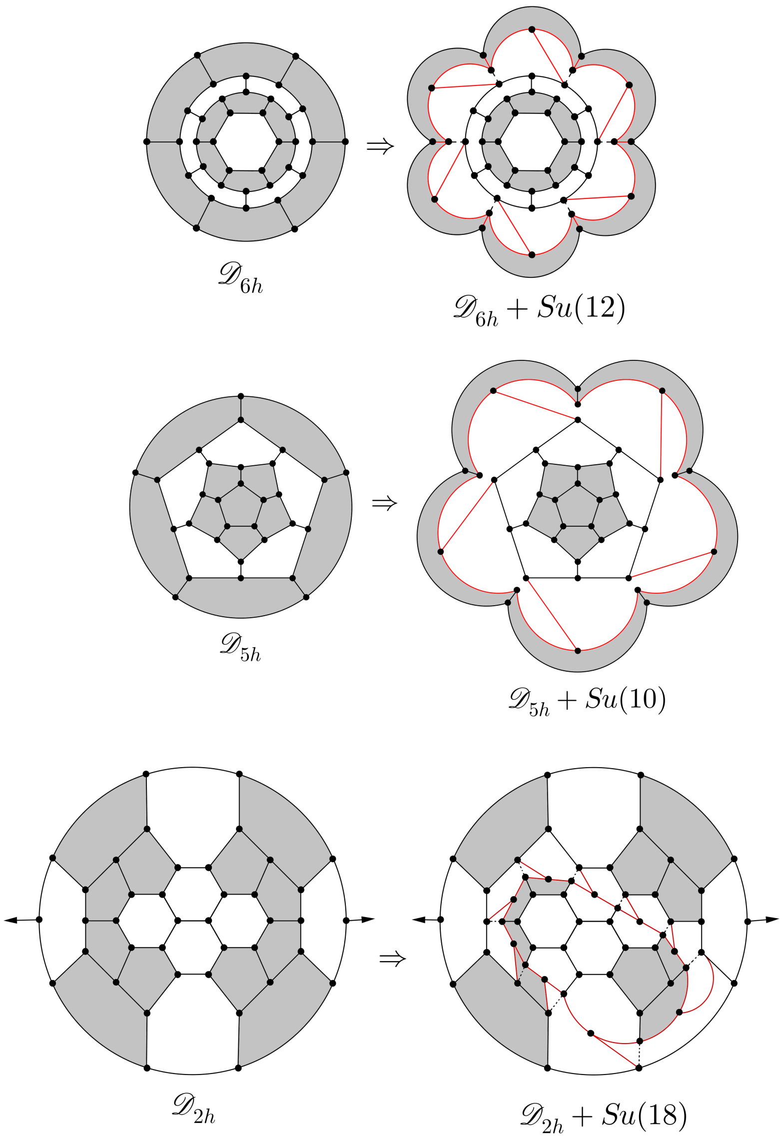


Figure 9: Some fullerenes with prismatic symmetry group generated by sun-shaped expansion.

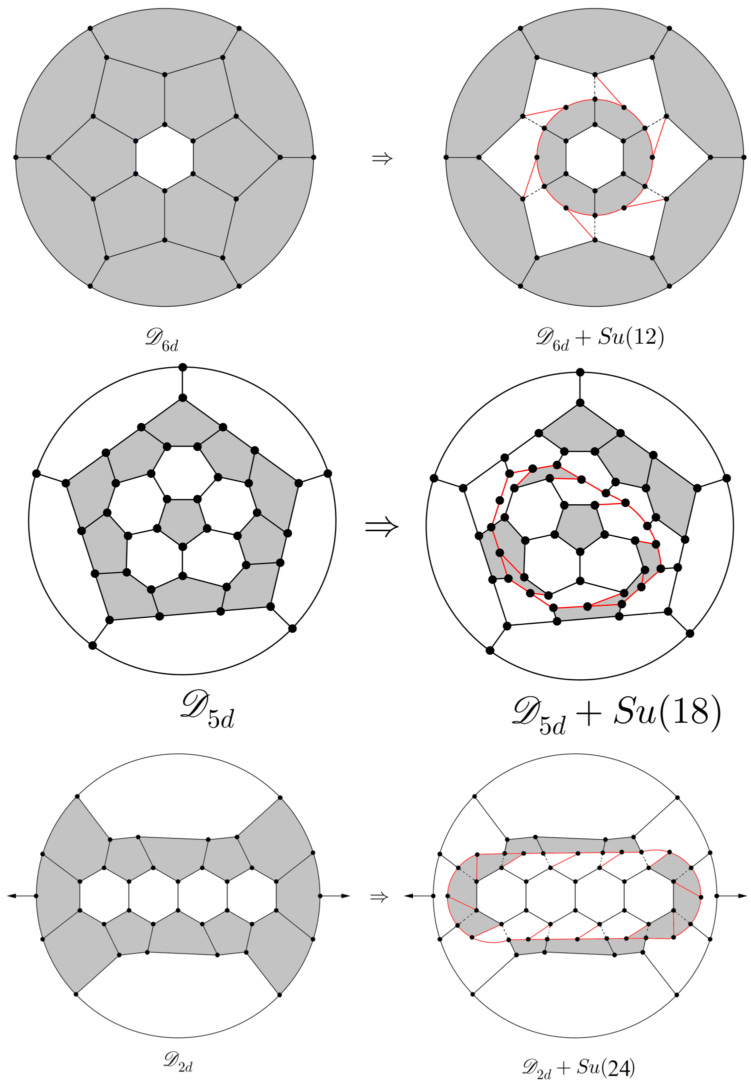


Figure 10: Some fullerenes with antiprismatic symmetry group generated by sun-shaped expansion.

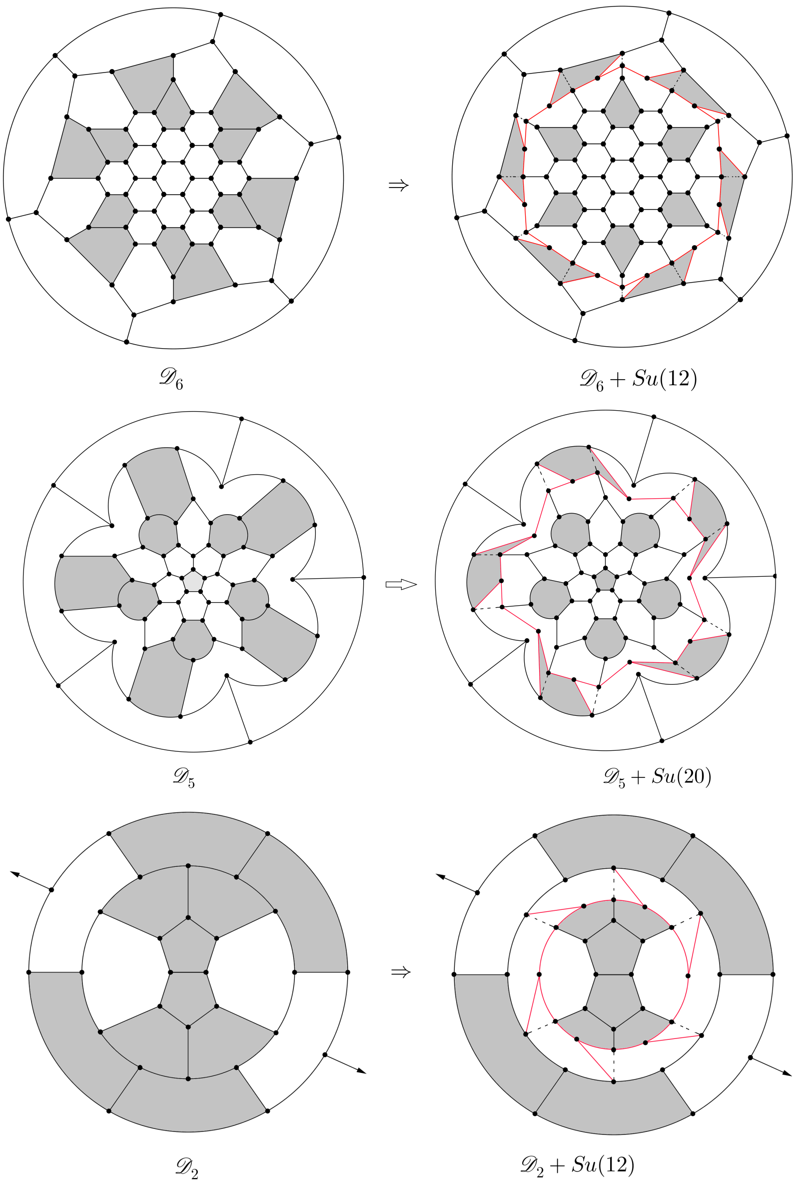


Figure 11: Some fullerenes with dihedral symmetry group generated by sun-shaped expansion.

Table 1: A list of fullerenes of various symmetry groups with related invariant.

Symmetry group	(F_b)	$\varphi(F_b)$	SSE(F_b)	$\varphi(SSE(F_b))$	$C_n(n \geq 2)$	$\varphi(C_n)$
prismatic	$\mathscr{D}_{6h}$	6	$\mathscr{D}_{6h} + Su(12)$	6	C_{36+12n}	6
	$\mathscr{D}_{5h}$	6	$\mathscr{D}_{5h} + Su(10)$	6	C_{30+10n}	6
	$\mathscr{D}_{2h}$	6	$\mathscr{D}_{2h} + Su(18)$	8	C_{40+18n}	8
antiprismatic	$\mathscr{D}_{6d}$	6	$\mathscr{D}_{6d} + Su(12)$	6	C_{24+12n}	6
	$\mathscr{D}_{5d}$	8	$\mathscr{D}_{5d} + Su(18)$	9	C_{40+18n}	7+2n
	$\mathscr{D}_{2d}$	6	$\mathscr{D}_{2d} + Su(24)$	6	C_{36+24n}	4+2n
dihedral	$\mathscr{D}_{6}$	6	$\mathscr{D}_{6} + Su(12)$	12	C_{48+12n}	12
	$\mathscr{D}_{5}$	8	$\mathscr{D}_{5} + Su(20)$	12	C_{60+20n}	12
	$\mathscr{D}_{2}$	6	$\mathscr{D}_{2} + Su(12)$	6	C_{28+12n}	6

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