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TOWARDS A PERIODIC PATTERN IN CLASSICAL AND NONCLASSICAL FULLERENES WITH TETRAHEDRAL STRUCTURE

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Abstract. We have considered the following classical fullerenes: C_{40} C_{84} and C_{92}. All of them have tetrahedral symmetry. The nonclassical fullerenes C_{64} and C_{76} were proposed earlier. Now, we have outlined a constructive process to obtain both fullerenes. The Table obtained earlier is complemented with four nonclassical fullerenes C_{52}, C_{60}, C_{88}, and C_{100}. The mass difference Δm between the numbers of carbon atoms of the fullerenes forms the sequence: 8, 4, 12, 8, 4, 12, 8, 4, 12. Its periodicity has no gaps as before.

Keywords: isolated pentagon rule, nonclassical fullerene, Schlegel diagram, tetrahedral symmetry

1. Introduction

Study of fullerenes has about three decades [1], where the faces of that kind of molecules were found to be hexagons and pentagons. Later, other polygons where considered [2]. Some work has focused upon certain geometric properties [3] as well as on considering types of symmetry [4,5] that can be analysed by using graph theory [6].

2. Tetrahedral structure

The first example that we consider is a classical fullerene that contains 40 carbons. We observe in Fig. 1 that at the central part of the molecule, there are three pentagons next to each other. This means that our fullerene does not satisfy the isolated pentagon rule (IPR).

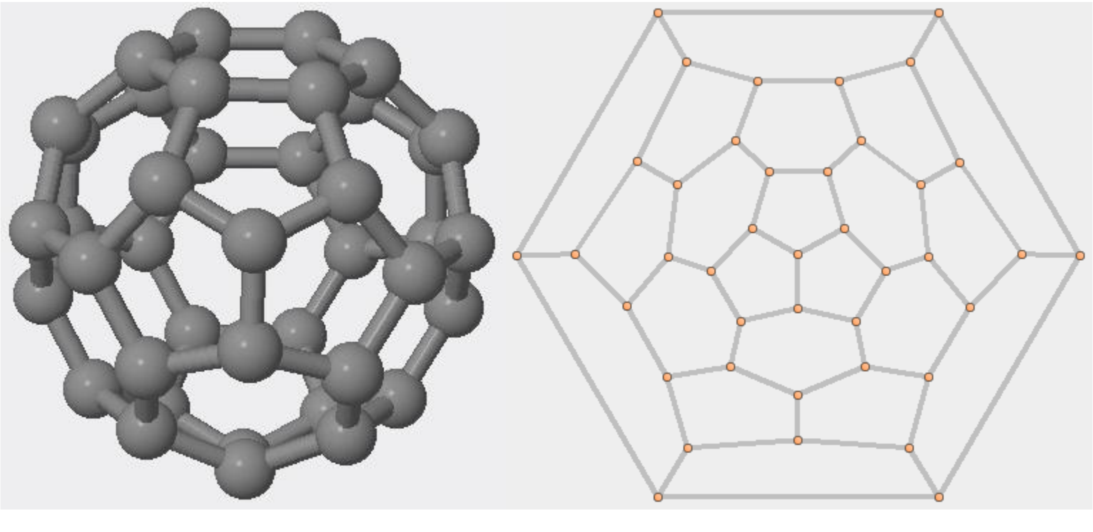

Fig. 1. Classical fullerene with 40 carbons (at the left) and its Schlegel diagram (at the right)

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In Schlegel diagram of fullerene C_{40}, we observe another group composed by three pentagons, located at the bottom of the graph, other group of three pentagons next to the right hand side corner of the graph, and other group of three pentagons next to the left hand side corner of the graph. Therefore, we have 12 pentagons and 10 hexagons.

The next fullerene contains 52 atoms, with 4 triangles, 12 pentagons, and 12 heptagons (Fig. 2). Each face of the structure is formed by one triangle surrounded by 3 heptagons, while vertices are constituted by 3 adjoined pentagons.

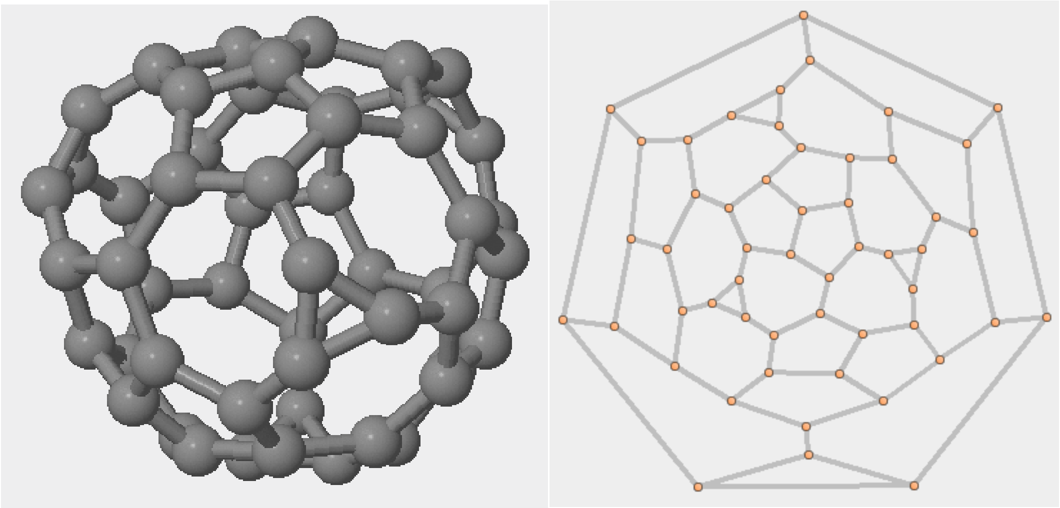

Fig. 2. Nonclassical fullerene C_{52} (at the left) and its Schlegel diagram (at the right)

The following fullerene contains 60 atoms, with 8 triangles, 12 hexagons and 12 heptagons (Fig. 3). Each face of the structure is formed by one triangle surrounded by 3 heptagons, while vertices are constituted by 3 adjoined hexagons with a triangle in the middle.

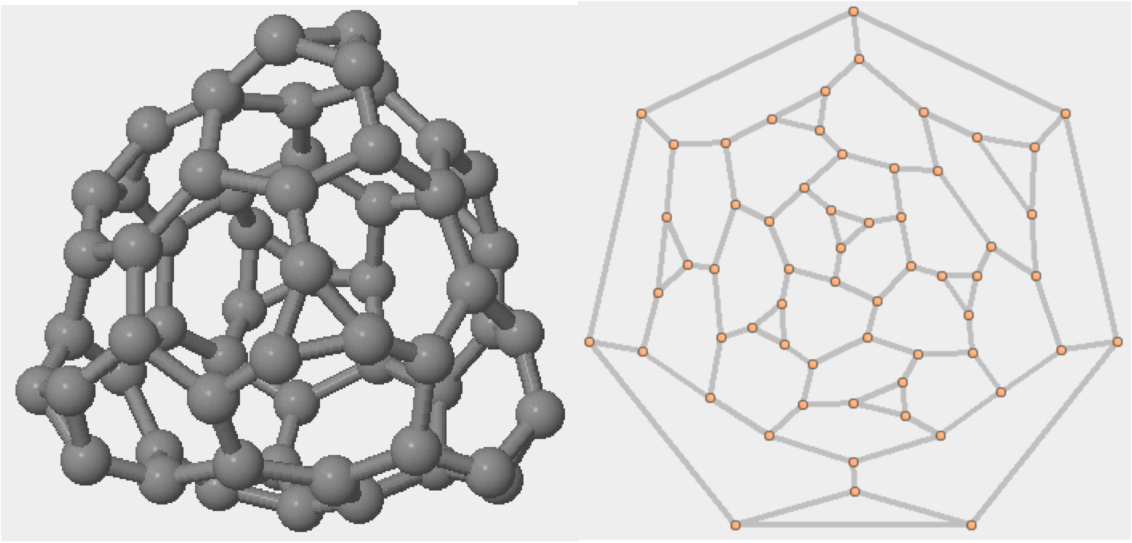

Fig. 3. Nonclassical fullerene C_{60} (at the left) and its Schlegel diagram (at the right)

Our next molecule of 64 atoms contains heptagons (Fig. 4). Thus, it is an example of a nonclassical fullerene. We have 64 carbons, 12 heptagons, 10 hexagons, and 12 squares. One face of C_{64} has 3 heptagons.

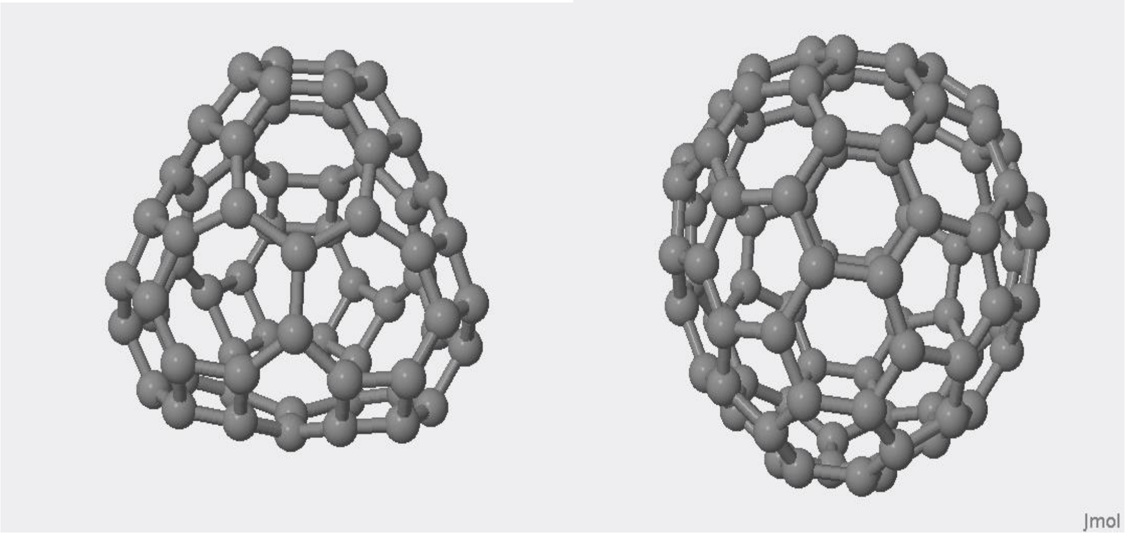

Fig. 4. Nonclassical fullerene C_{64} (at the left) and classical fullerene C_{84} (at the right)

In order to obtain the nonclassical fullerene C_{64}, consider the C_{84} classical isomer with tetrahedral structure, and then replace the seven hexagons located next to each other (that form a face) by three heptagons. The original face has 12 inner carbons, and the new face contains 10 inner carbons. Therefore, after this first step, a nonclassical fullerene with 82 carbons is generated, which is shown in Fig. 5 at the left.

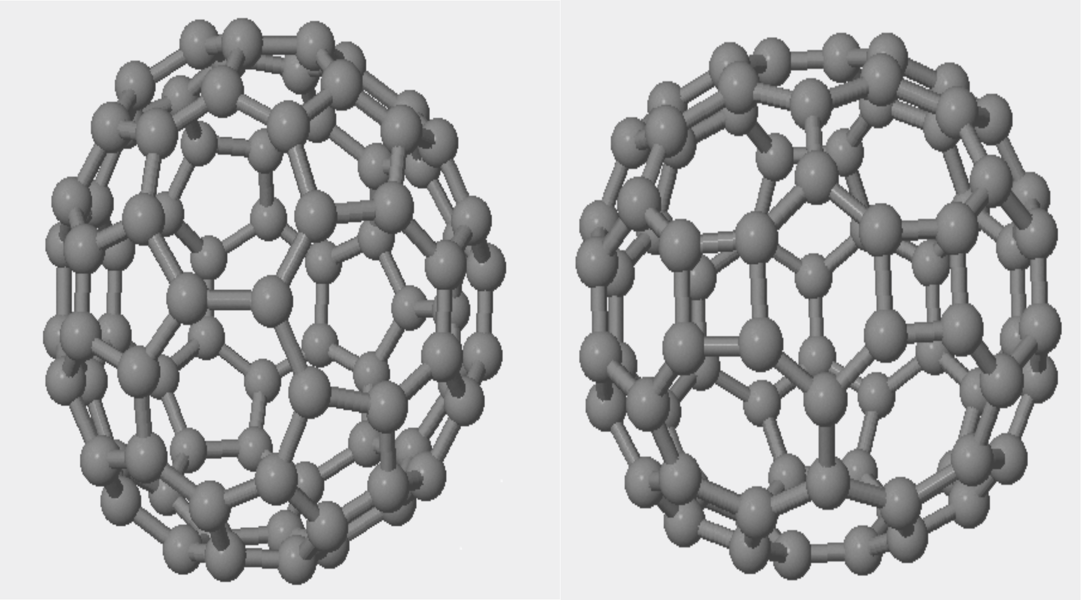

Fig. 5. Nonclassical fullerene with 82 carbons (at the left) and fullerene with 78 carbons (at the right)

Moreover, in Fig. 5 one can observe that between the new face and the original ones, a pentagon takes the place of a previous hexagon. After we replace another face of seven hexagons by three heptagons we obtain a nonclassical fullerene with 78 carbons (Fig. 5, at the right).

Meanwhile, on Schlegel diagram (Fig.6, at the left) we have a couple of squares. Next, we repeat this procedure for the third time to obtain a nonclassical fullerene with 72 carbons which is shown in Fig. 6, at the right. Finally, after the last iteration, we have the nonclassical fullerene with 64 carbons presented in Fig. 4, at the left.

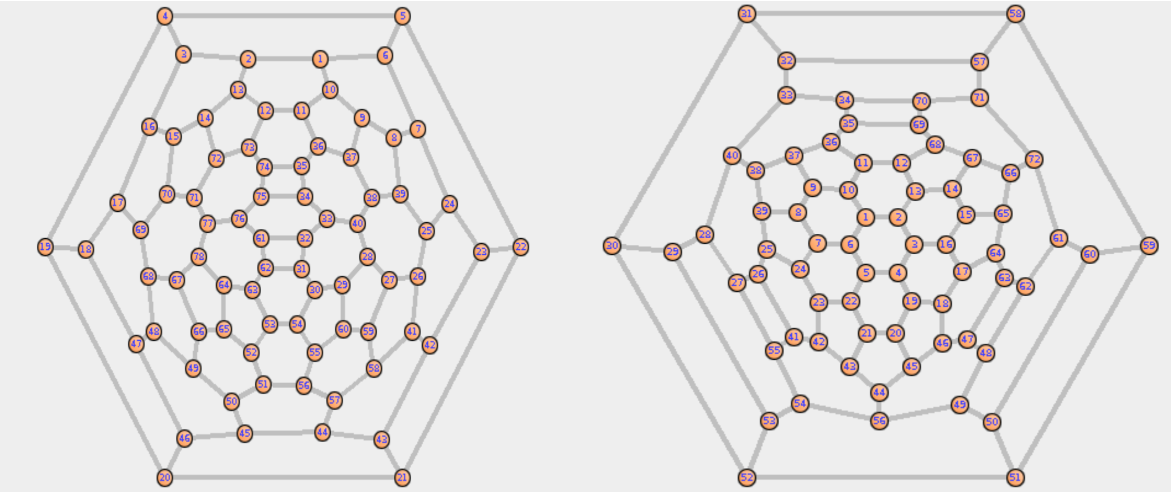

Fig. 6. Fullerene of 78 atoms (at the left) and nonclassical fullerene of 72 atoms (at the right)

In our previous construction, the faces formed by three heptagons, have hexagons as vertexes, and between two hexagons there is a boundary filled out with one hexagon and two squares. But, if this boundary consists of four pentagons, instead of squares and the hexagon, for each of the six boundaries, we have two additional carbons, which give 12 more carbons. Therefore, we obtain a new nonclassical fullerene with 64 + 12 = 76 carbons, which is shown in Fig. 7, at the left, and the corresponding Schlegel diagram presented in Fig. 7, at the right.

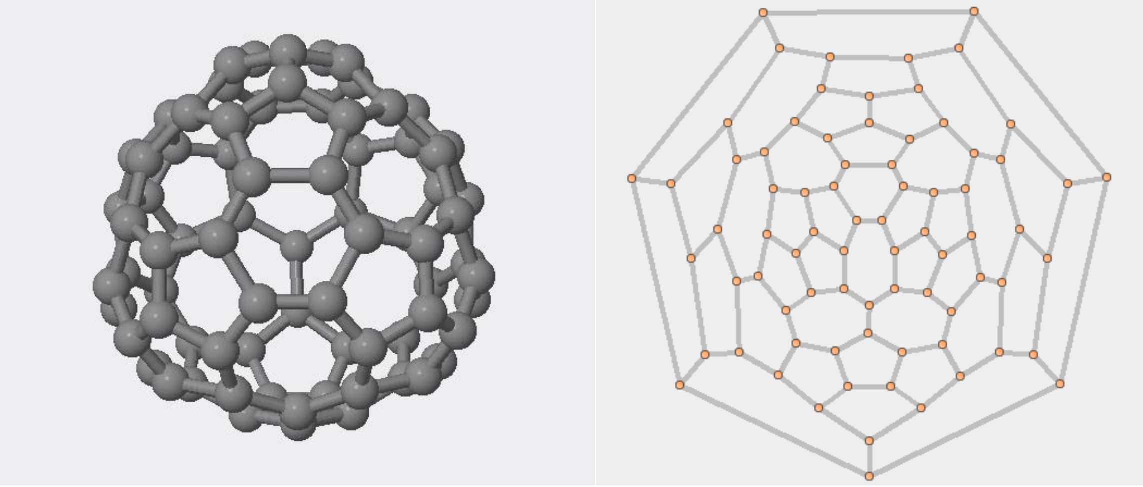

Fig. 7. Fullerene with 76 carbons (at the left) and its Schlegel diagram (at the right)

Now we consider a fullerene with 88 carbons, containing 6 octagons (Fig. 8). We observe four corners constituted by one hexagon surrounded by six pentagons. Then we have 12 hexagons coming from the four faces, plus 4 more hexagons from the corners, giving a total of 16 hexagons. Now we take into account 24 pentagons from the four corners, and 6 octagons.

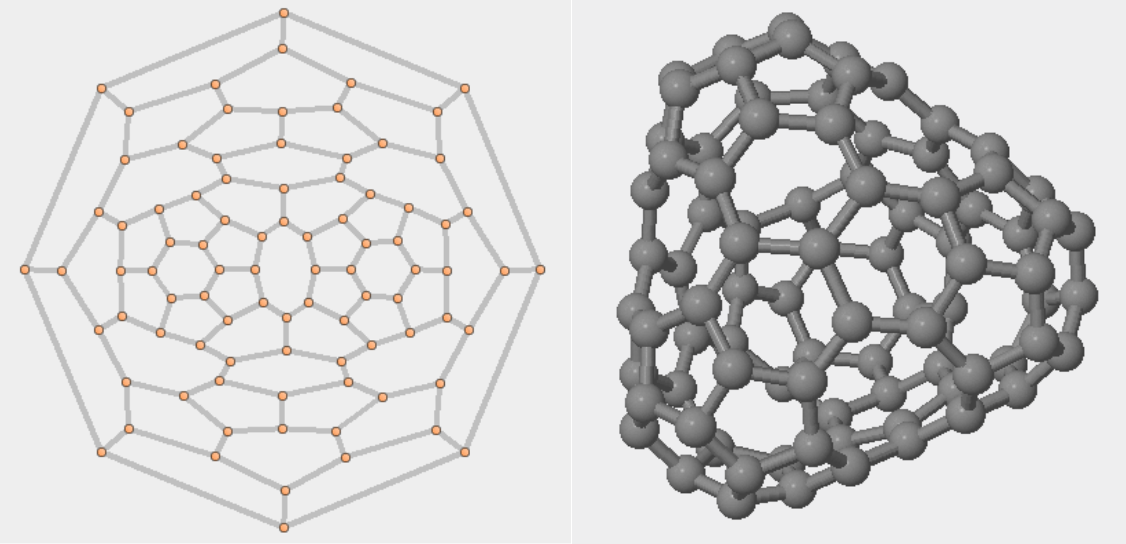

Fig. 8. Schlegel diagram of C_{88} (at the left) and the corresponding nonclassical fullerene (at the right)

Now, as an intermediate step, consider the classical fullerene with 92 carbons having a tetrahedral structure (Fig. 9). Each face of this fullerene is formed by three adjoined hexagons that have only one node in common. These three hexagons are surrounded by three pentagons.

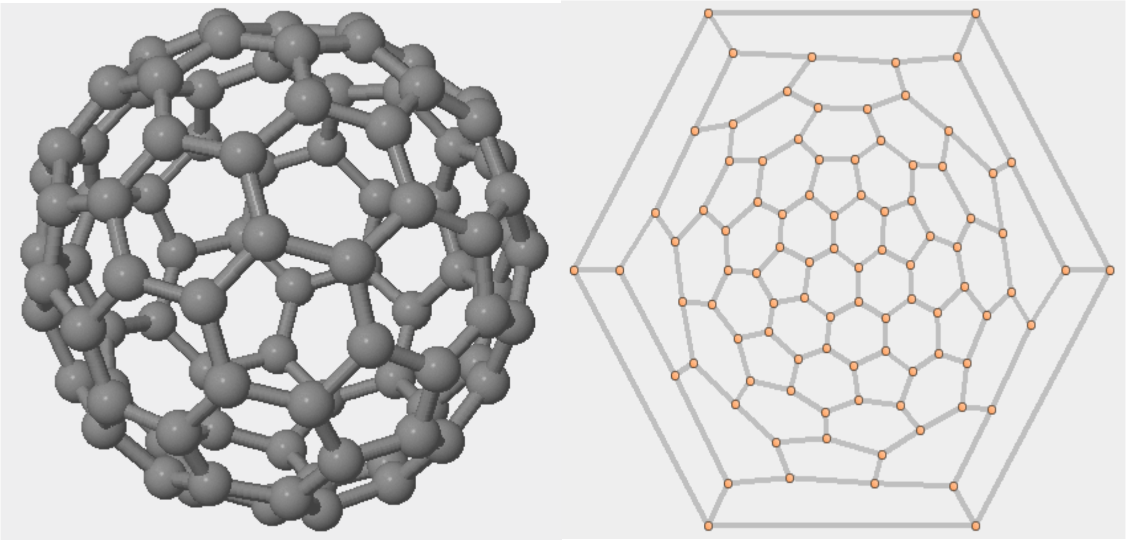

Fig. 9. Face of classical fullerene C_{92} (at the left) and Schlegel diagram of C_{92} (at the right)

The three hexagons will be replaced by three heptagons and one triangle in the middle. We add three nodes by face and delete the node at the middle. Hence we have two new nodes by face, and there are 4 faces. In consequence, we have 8 additional nodes (Fig. 10).

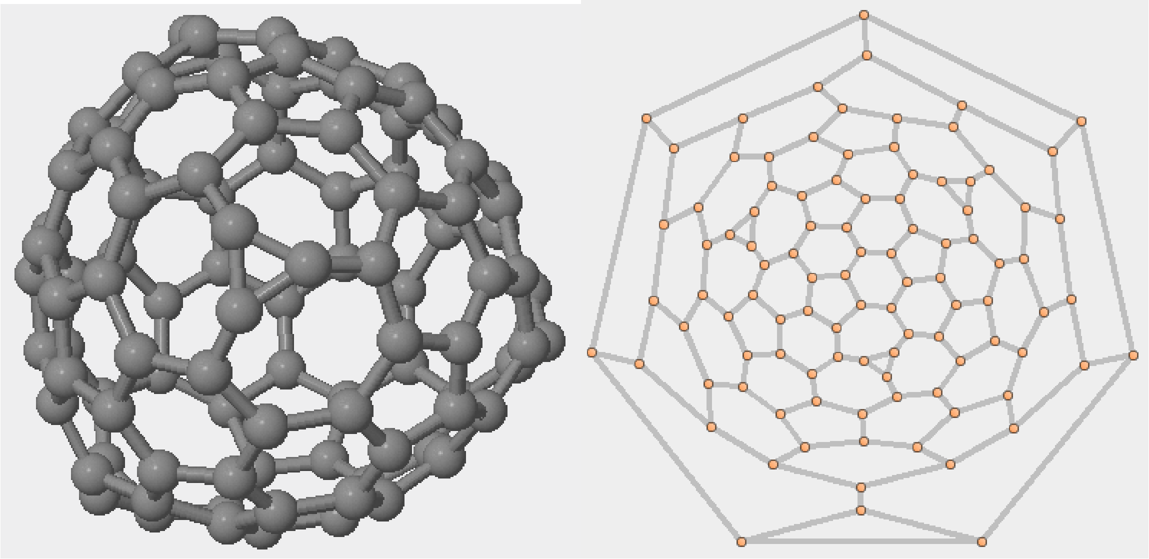

Fig. 10. Face of nonclassical fullerene C_{100} (at the left) and Schlegel diagram of C_{100} (at the right)

3. Structural analysis

Study of tetrahedral mini- and midi-fullerenes is achieved in [6] where a Table with fullerenes C_4, C_{12}, C_{16}, C_{28}, C_{36}, C_{64} and C_{76} is presented. Fullerenes with 64 and 76 carbons are the same that are considered in this work. As the authors comment, there are some gaps in the Table when the differences between the numbers of fullerene carbons are taken into account. Let us see what happens if we add to the Table several fullerenes, namely C_{40}, C_{52}, C_{60}, C_{84}, C_{88}, and C_{100}. Here we follow the type of graphs displayed in [6]. Then the structure of these added fullerenes looks as follows.

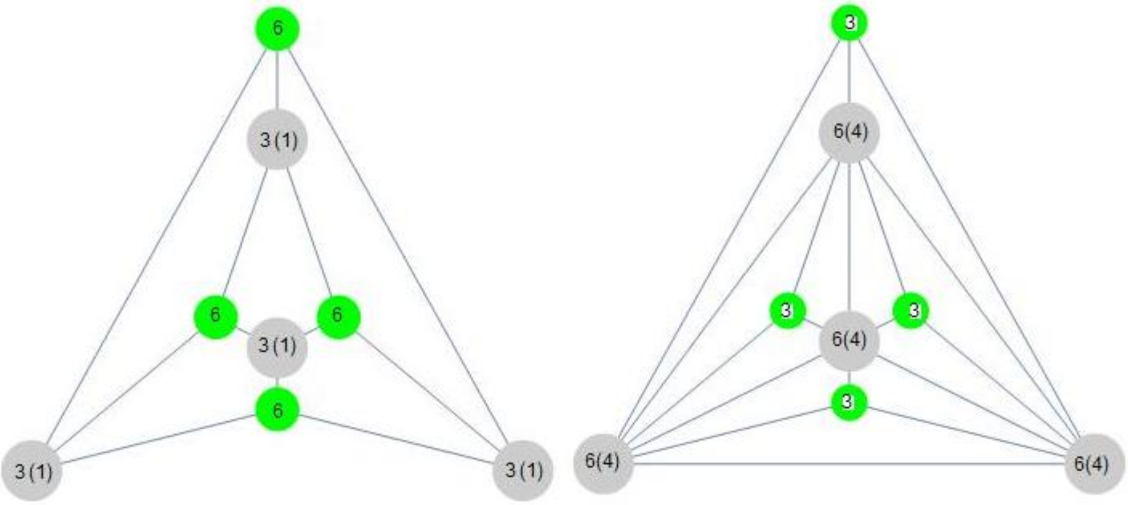

Fig. 11. Structure of fullerene C_{40} at the left and that of fullerene C_{52} at the right

It should be mentioned that classical fullerene C_{84} was initially considered as an initial step constructing the nonclassical fullerene C_{64}, but now this fullerene C_{84} of tetrahedral symmetry is going to be one part on completing the Table presented in [6].

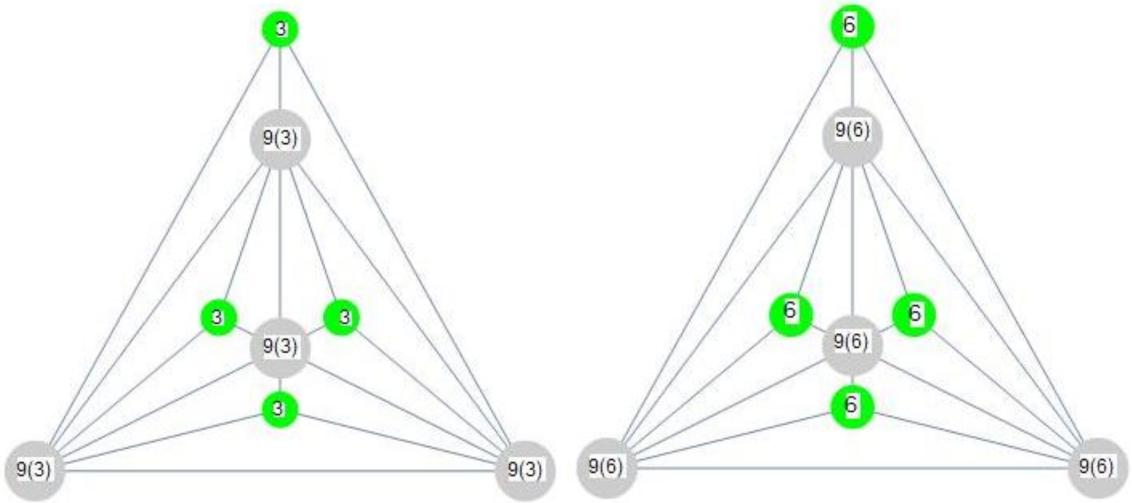

Fig. 12. Structure of fullerene C_{60} at the left and that of fullerene C_{84} at the right

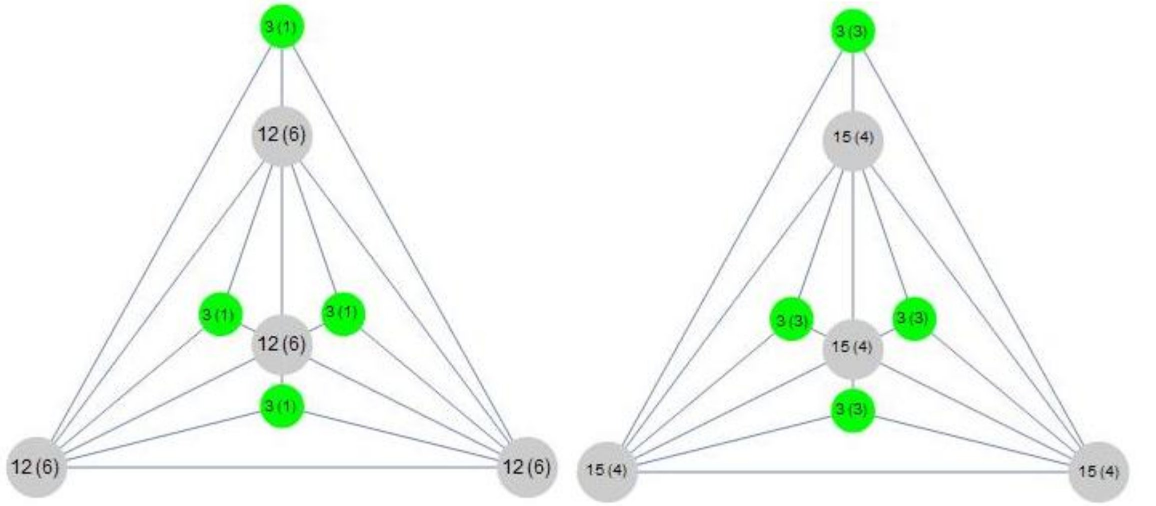

Fig. 13. Structure of fullerene C_{88} at the left and that of nonclassical fullerene C_{100} at the right

Table 1. List of considered fullerenes with Tetrahedral symmetry

Fullerenes	Chemical formula	Number of atoms
C_4	A_1	4 (1) = 4
C_{12}	B_3	4 (3) = 12
C_{16}	A_1 B_3	4 (1 + 3) = 16
C_{28}	A_1 B_6	4 (1 + 6) = 28
C_{36}	A_3 B_6	4 (3 + 6) = 36
C_{40}	A_6 B_3 (C_1)	4 [6 + (3 + 1)] = 40
C_{52}	A_3 B_6 (C_4)	4 [3 + (6 + 4)] = 52
C_{60}	A_3 B_9 (C_3)	4 [3 + (9 + 3)] = 60
C_{64}	A_3 (C_1) B_6 (C_6)	4 [(3 + 1) + (6 + 6)] = 64
C_{76}	A_3 (C_1) B_9 (C_6)	4 [(3 + 1) + (9 + 6)] = 76
C_{84}	A_9 B_6 (C_6)	4 [(9 + 6) + 6] = 84
C_{88}	A_3 (C_1) B_{12} (C_6)	4 [(3 + 1) + (12 + 6)] = 88
C_{100}	A_3 (C_3) B_{15} (C_4)	4 [(3 + 3) + (15 + 4)] = 100

4. Discussion

We have considered the following classical fullerenes: C_{40} (that does not satisfy the isolated pentagon rule), C_{84} and C_{92} (as an initial step to obtain the nonclassical fullerene C_{100}). All of them have tetrahedral symmetry. As it was mentioned before, the nonclassical fullerenes C_{64} and C_{76} were proposed in [4]. Now, we have outlined a constructive process to obtain both fullerenes. The Table obtained earlier is complemented with three nonclassical fullerenes C_{52}, C_{60}, C_{88}, and the already mentioned C_{100}.

If we compute the mass difference Δm between the numbers of carbon atoms of the fullerenes in the Table 1, the sequence 8, 4, 12, 8, 4, 12, 8, 4, 12 is obtained. It has the periodicity without gaps as in the Table obtained earlier [6].

Future work will be focused in trying to extend this pattern to fullerenes of tetrahedral symmetry that contain more atoms.

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