ON SOME EXAMPLES OF FULLERENES WITH HEPTAGONAL RINGS

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ABSTRACT

Several works on nonclassical fullerenes with heptagons have mainly considered the case with just one heptagon. In this context the isolated pentagon rule is not satisfied. The study of nonclassical fullerenes is important because some of them are more stable than the corresponding classical isomers with the same number of pentagonal bonds. We present several nonclassical fullerenes with pentagons, hexagons and two, three, or more heptagons.

Keywords: *Fullerene, heptagon, pentagon adjacency penalty rule, Euler's polyhedron formula.*

1. INTRODUCTION

Classical fullerenes are those carbon cage molecules with exactly 12 pentagons and $n/2 - 10$ hexagons, Patrick Fowler and David Manolopoulos [1]. All classical fullerenes satisfy the so called isolated pentagon rule IPR, Harold Kroto [2]. On the other hand, nonclassical fullerenes are those carbon cage molecules embedded with one or more squares or heptagons. In this last case, sometimes pentagon-pentagon adjacencies appear, and the most stable structure allows for the least pentagon-pentagon adjacencies, which is known as the pentagon adjacency penalty rule PAPR, Eleanor Campbell *et al* [3]. Actually, the IPR or PAPR has been an efficient criterion for explaining the stability of fullerenes.

2. BACKGROUND

An amount of work has been done to study nonclassical fullerenes. For instance, Andrés Ayuela *et al* [4] show theoretical evidence for the existence of a nonclassical fullerene C_{62} with one heptagonal, 13 pentagonal and 19 hexagonal rings. Jie An *et al* [5] study the isomers of fullerene C_{26} composed of square, pentagonal, hexagonal, and heptagonal faces. Yuan-Zhi Tan *et al* [6] consider the fullerene C_{68} which contains one heptagonal ring. Furthermore, Li-Hua Gan *et al* [7] study fullerenes C_{46}, C_{48}, C_{50}, and C_{52}, some of them composed of one heptagonal ring.

3. CALCULATIONS

We have obtained the graphs of our results by running the V0.3 version of (Carbon Generator) CaGe software, Gunnar Brinkmann [8], [9]. Schlegel diagrams [10] are also provided for each considered fullerene.

Our first example of nonclassical fullerene contains 68 carbons with two heptagonal rings, 14 pentagons, and 20 hexagons. Therefore, this polyhedron has a total number of 36 faces, 102 edges, and of course 68 vertexes. It is shown the 2-dimensional representation (Schlegel diagram) of this fullerene in Figure 1, and its 3-dimensional graph in Figure 2.

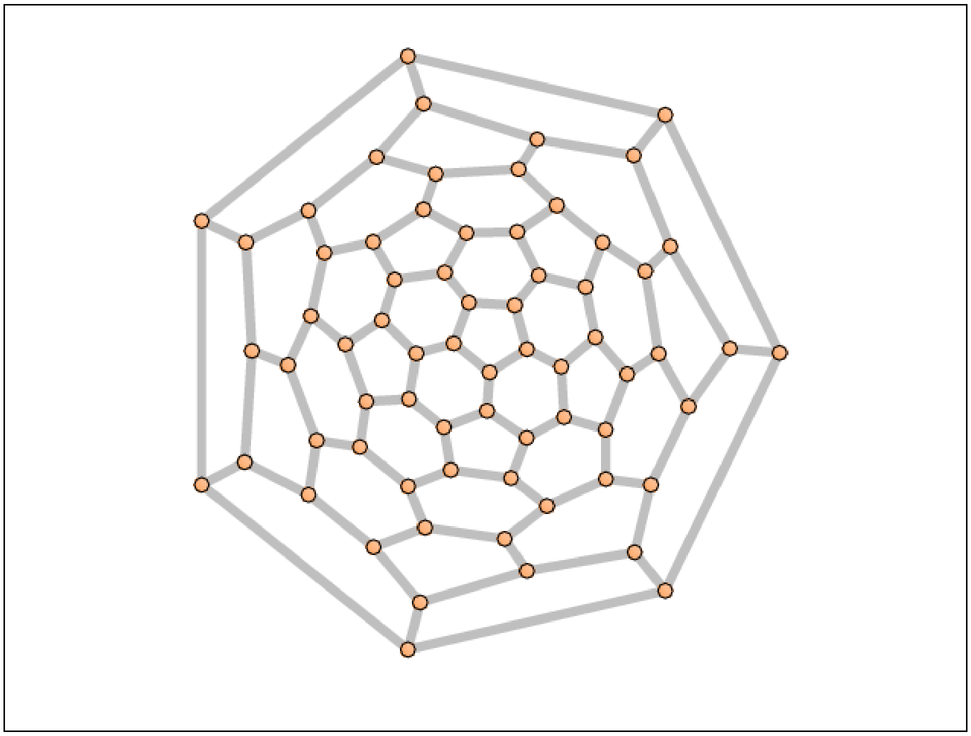

Figure 1. Schlegel diagram for the 68 carbons fullerene.

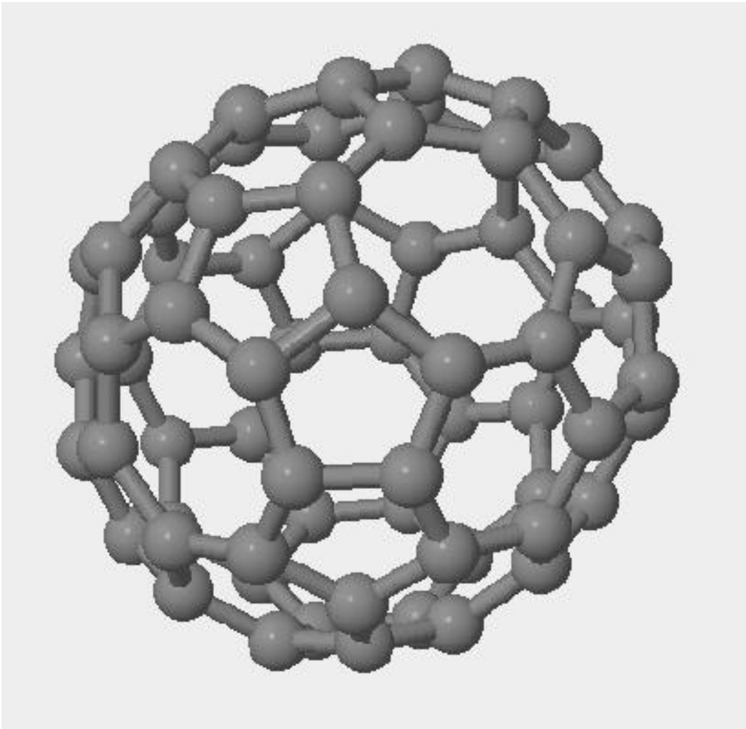

Figure 2. Fullerene with 68 carbons, 2 heptagons,
20 hexagons, and 14 pentagons.

The second example of nonclassical fullerene has 80 carbons, three heptagonal rings, 15 pentagons, and 24 hexagons. This polyhedron has a total number of 42 faces, 120 edges, and of course 80 vertexes. The Schlegel diagram of this fullerene is shown in Figure 3, and its 3-dimensional graph in Figure 4.

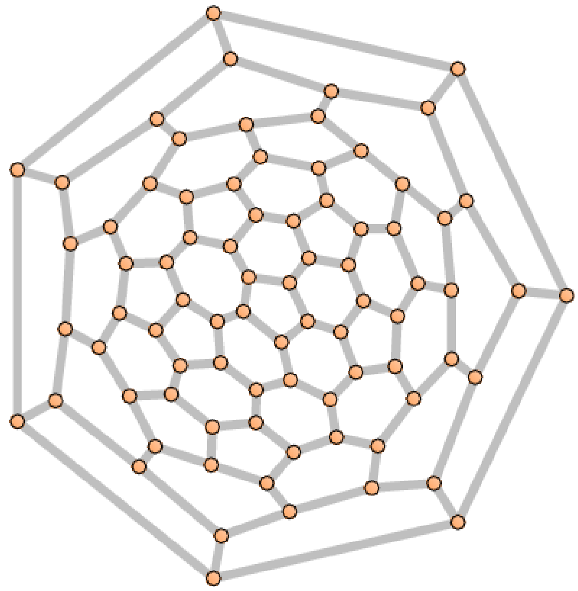

Figure 3. Schlegel diagram for the 80 carbons fullerene.

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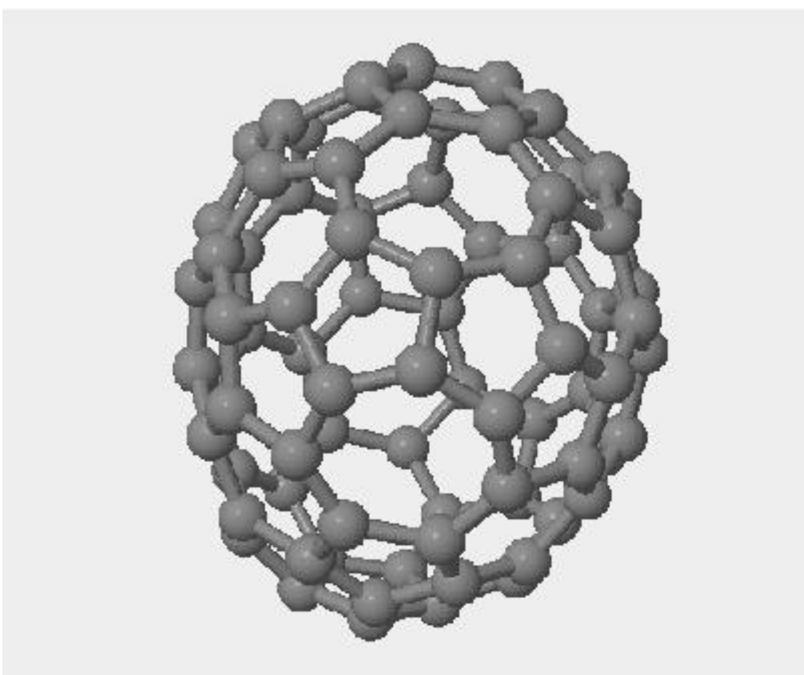

Figure 4. Fullerene with 80 carbons, 3 heptagons, 24 hexagons, and 15 pentagons.

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Next, the third example of nonclassical fullerene contains 82 carbons with four heptagonal rings, 16 pentagons, and 23 hexagons. Therefore, this polyhedron has a total number of 43 faces, 123 edges, and of course 82 vertexes. It is shown the 2-dimensional representation of this fullerene in Figure 5, and its 3-dimensional graph in Figure 6.

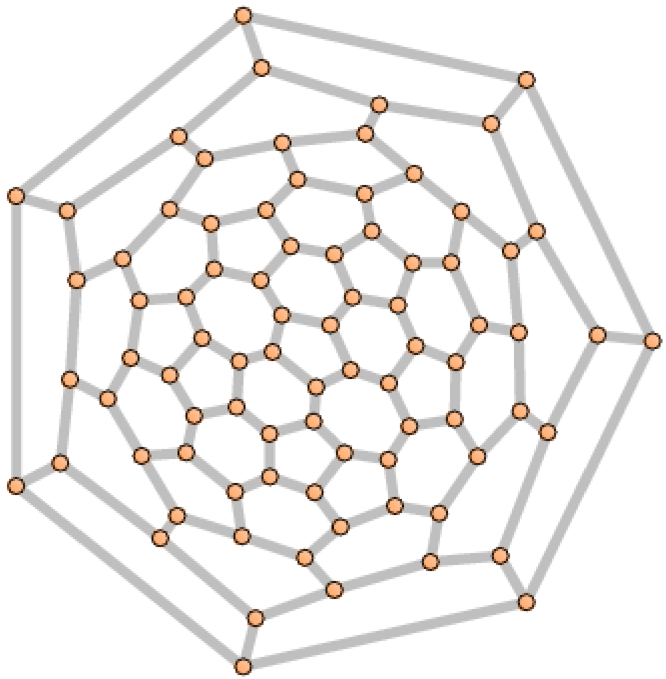

Figure 5. Schlegel diagram for the 82 carbons fullerene.

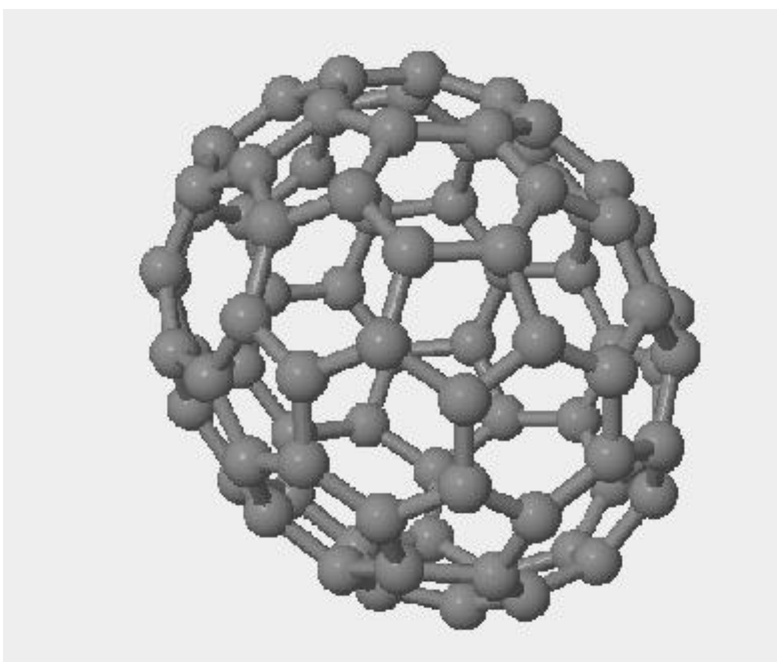

Figure 6. Fullerene with 82 carbons, 4 heptagons, 23 hexagons, and 16 pentagons.

The fourth example of nonclassical fullerene contains 76 carbons with six heptagonal rings, 18 pentagons, and 16 hexagons. Therefore, this polyhedron has a total number of 40 faces, 114 edges, and of course 76 vertexes. The 2-dimensional representation of this fullerene is shown in Figure 7, and its 3-dimensional graph in Figure 8.

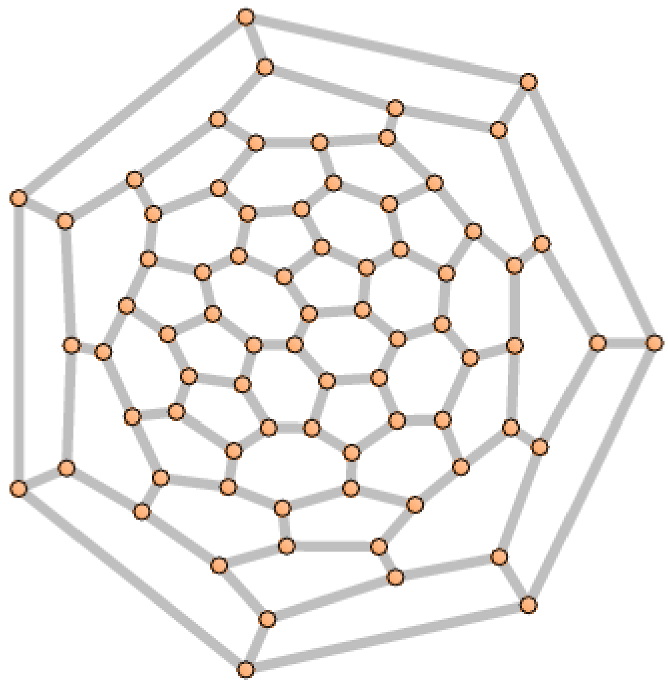

Figure 7. Schlegel diagram for the 76 carbons fullerene.

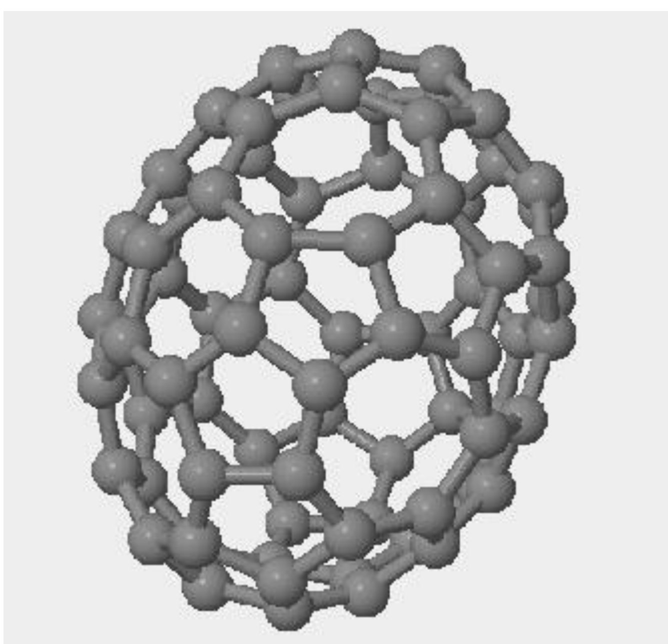

Figure 8. Fullerene with 76 carbons, 6 heptagons, 16 hexagons, and 18 pentagons.

Next, the fifth example of nonclassical fullerene contains 64 carbons with five heptagonal rings, 17 pentagons, and 12 hexagons. Therefore, this polyhedron has a total number of 34 faces, 96 edges, and of course 64 vertexes. It is shown the 2-dimensional representation of this fullerene in Figure 9, and its 3-dimensional graph in Figure 10.

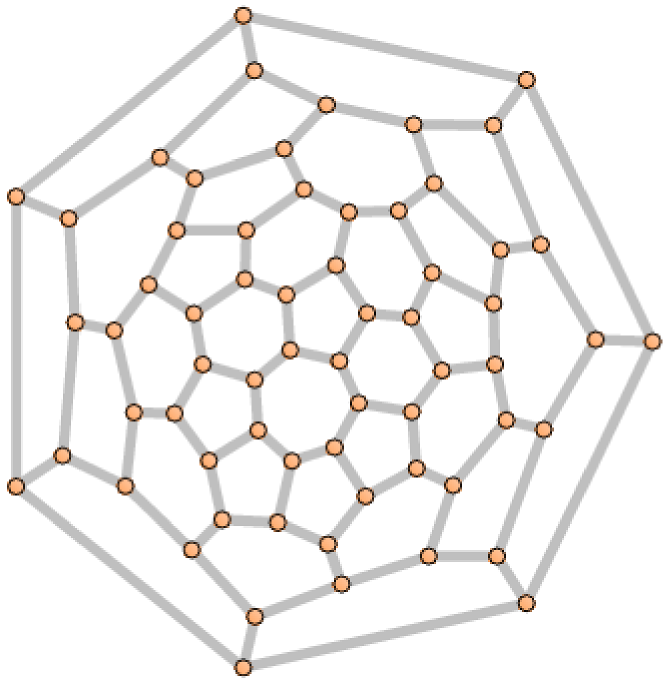

Figure 9. Schlegel diagram for the 64 carbons fullerene.

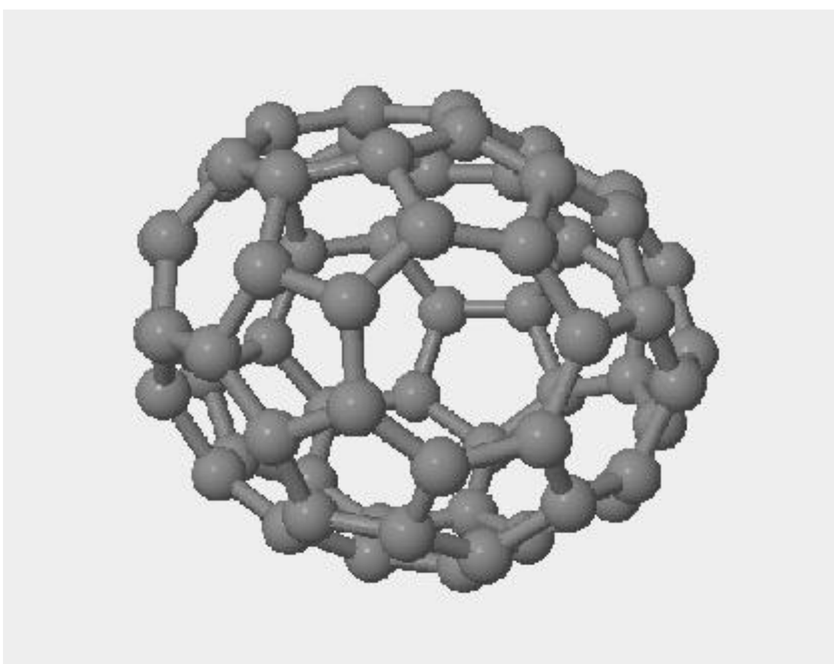

Figure 10. Fullerene with 64 carbons, 5 heptagons, 12 hexagons, and 17 pentagons.

Our last example of nonclassical fullerene contains 42 carbons with two heptagonal rings, 14 pentagons, and 7 hexagons. Therefore, this polyhedron has a total number of 23 faces, 63 edges, and of course 42 vertexes. The 2-dimensional representation of this fullerene is shown in Figure 11, and its 3-dimensional graph in Figure 12. By the way, a complete reference about numerical procedures on Nanoscience, can be found in [11].

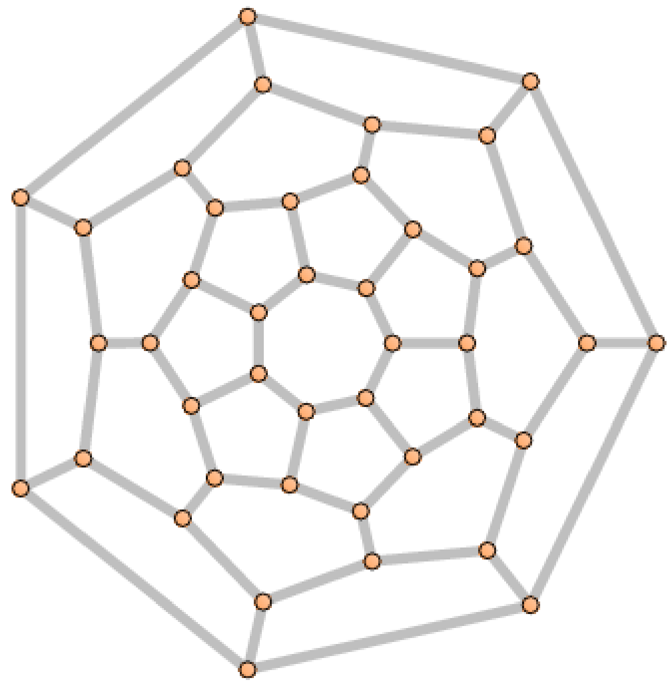

Figure 11. Schlegel diagram for the 42 carbons fullerene.

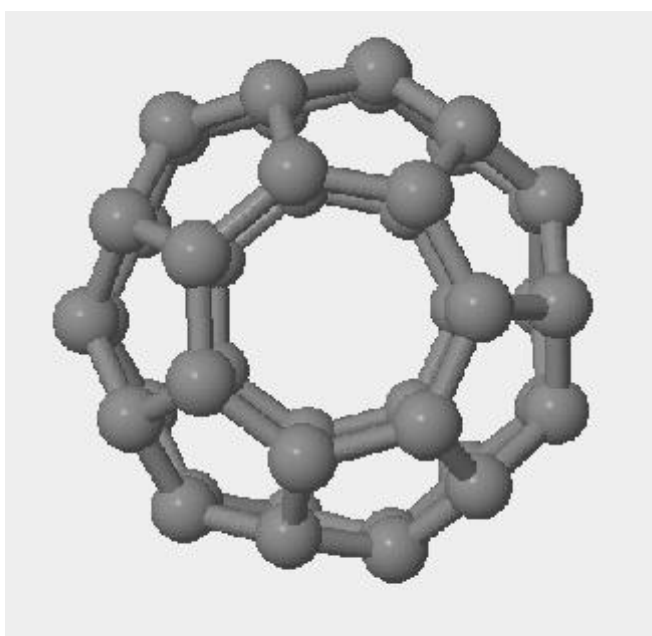

Figure 12. Fullerene with 42 carbons, 2 heptagons, 7 hexagons, and 14 pentagons.

4. CONCLUSIONS

We have considered six nonclassical fullerenes with two, three, four, five, and six heptagonal rings. In the case of the 68 carbons fullerene, it contains 2 heptagonal rings. One of them is surrounded by 4 pentagons next to each other, and one pentagon lies between 2 hexagons. The other heptagonal ring is surrounded by a couple of pentagons, which lies between two hexagons; the border is completed by one hexagon in the middle of 2 pentagons. With respect to the 80 carbons case, the structure of the pentagons and hexagons surrounding each one of the 3 heptagonal rings follows one of the patrons of the 68 carbons fullerene. A similar situation occurs with the 82 carbons case. But, the 76 carbon fullerene, presents two new cases: a couple of pentagons, then a hexagon, followed by another couple of pentagons, and the boundary of this heptagonal ring is completed by 2 hexagons next to each other. The other type boundary surrounding a heptagonal ring is: a couple of hexagons, which lie between two pentagons; the border is completed by one pentagon in the middle of 2 hexagons. Another case appears on the 64 carbons fullerene: each one of two heptagonal rings are surrounded by 6 pentagons and only one hexagon. Finally, the most extreme case is observed on the 42 carbons fullerene, where the heptagons are bounded by 7 pentagons.

5. ACKNOWLEDGEMENTS

The authors thanks Berenice Sánchez and Óscar del Valle for installation of CaGe software.

6. REFERENCES

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