Fullerenes with Heptagonal Rings An Overview

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***Abstract*— Several works on nonclassical fullerenes with heptagons have mainly considered the case with just one heptagon. 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.**

I. INTRODUCTION

Classical fullerenes are those carbon cage molecules with exactly 12 pentagons and *n/2 - 10* hexagons, Fowler and Manolopoulos [1]. All classical fullerenes satisfy the so called isolated pentagon rule IPR, 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, Campbell *et al* [3].

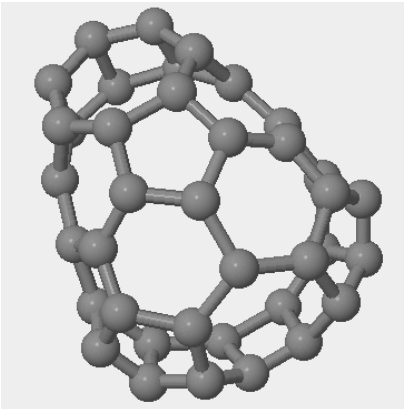

FIGURE 1. MOLECULE WITH 38 CARBONS, 2 HEPTAGONS, 4 HEXAGONS, AND 7 PENTAGONS, AND 7 SQUARES.

II. 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 fulle-

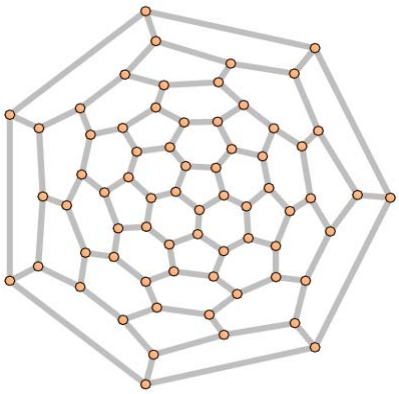

FIGURE 2. SCHLEGEL DIAGRAM FOR THE 68 CARBONS FULLERENE.

rene 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.

III. CALCULATIONS

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

Raghavachari *et al* [9] consider some corannulene-like form (bowl) of carbon molecules. Thus, inspired by that models, we present a preliminary example on Figure 1 with 38 carbons, 20 faces, and 56 edges.

We can observe in Figure 1 that, as it was mentioned previously besides heptagons, some nonclassical fullerenes may contain squares, and even octagons: Xian-Lei Sheng *et al* [10].

Our first real example of a nonclassical fullerene contains 68 carbons with two heptagonal rings, 14 pentagons, and 20 he- xagons. Therefore, this polyhedron

has a total of 36 faces, 102 edges, and of course 68 vertexes.

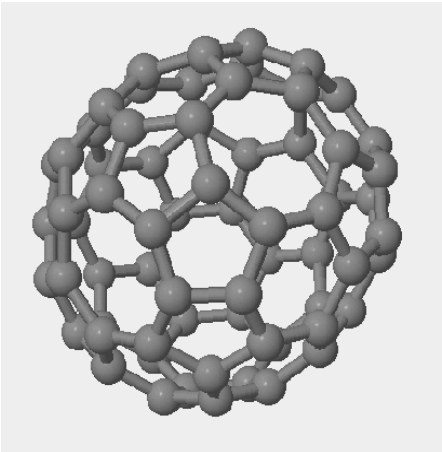

FIGURE 3. FULLERENE WITH 68 CARBONS, 2 HEPTAGONS, 20 HEXAGONS, AND 14 PENTAGONS.

It is shown the 2-dimensional (Schlegel diagram) of this fullerene, and its 3-dimensional graph in Figure 2 and 3, respectively.

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 4, and its 3-dimensional graph in Figure 5.

Next, the third example of nonclassical fullerene contains 82 carbons with four heptagonal rings, 16 pentagons, and 23 hexagons. Thus, this polyhedron has a number of 43 faces, 123 edges, and of course 82 vertexes. It is shown the 2-dimensional representation of this fullerene in Figure 6, and its 3-dimensional graph in Figure 7.

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 8, and its 3-dimensional graph in Figure 9.

Finally, 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 10, and its 3-dimensional graph in Figure 11.

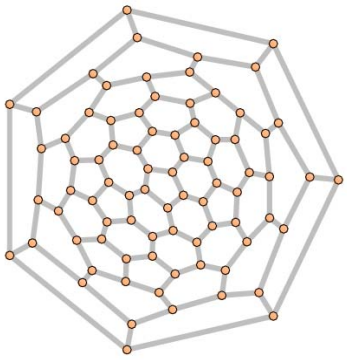

FIGURE 4. SCHLEGEL DIAGRAM FOR THE 80 CARBONS FULLERENE.

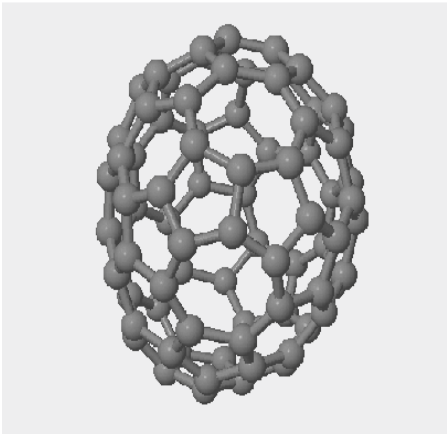

FIGURE 5. FULLERENE WITH 80 CARBONS, 3 HEPTAGONS, 24HEXAGONS, AND 15 PENTAGONS.

CONCLUSIONS

We have considered five nonclassical fullerenes with two, three, four, five, and six heptagonal rings. In the case of the 68 carbons fullerene, it contains 2 heptagonal rings.

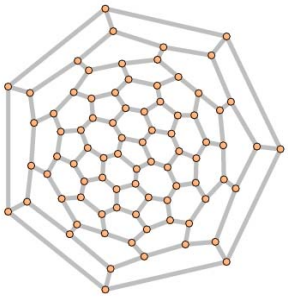

FIGURE 6. SCHLEGEL DIAGRAM FOR THE 82 CARBONS FULLERENE.

One of them is surrounded by 4 pentagons next to each other, and one pentagon lies between 2 hexagons.

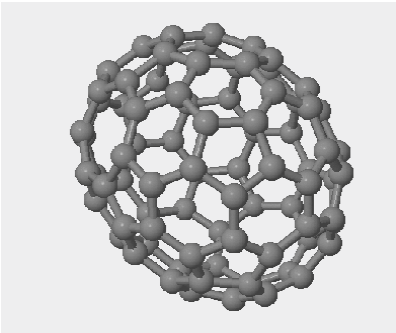

FIGURE 7. FULLERENE WITH 82 CARBONS, 4 HEPTAGONS, 23HEXAGONS, AND 16 PENTAGONS.

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.

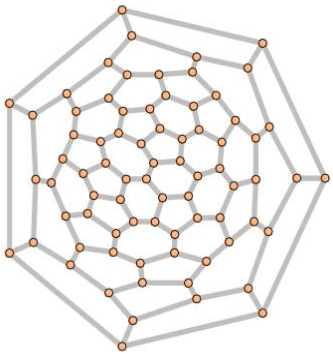

FIGURE 8. SCHLEGEL DIAGRAM FOR THE 76 CARBONS FULLERENE.

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.

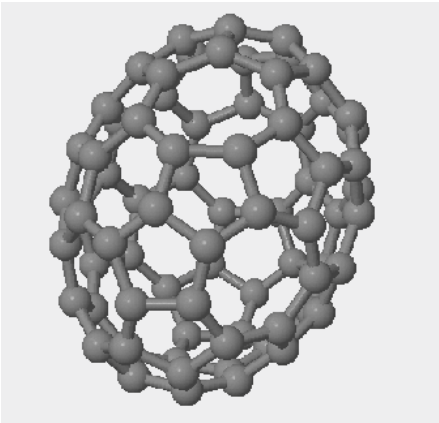

FIGURE 9. FULLERENE WITH 76 CARBONS, 6 HEPTAGONS, 16 HEXAGONS, AND 18 PENTAGONS.

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.

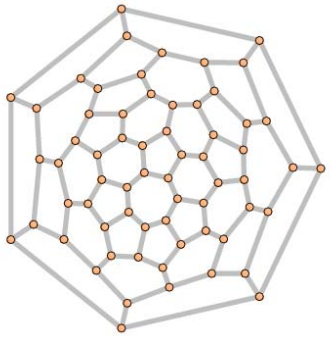

FIGURE 10. SCHLEGEL DIAGRAM FOR THE 64 CARBONS FULLERENE.

Finally, another case appears on the 64 carbons fullerene: each one of two heptagonal rings are surrounded by 6 pentagons and only one hexagon.

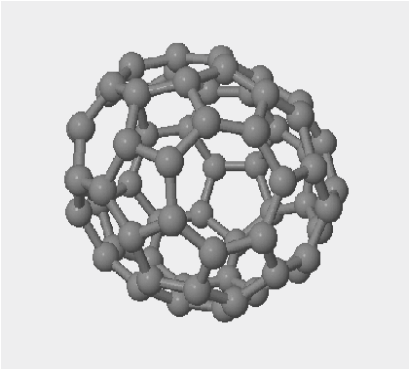

FIGURE 11. FULLERENE WITH 64 CARBONS, 5 HEPTAGONS, 12 HEXAGONS, AND 17 PENTAGONS.

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