Study of Nonclassical Fullerenes C_{192} and C_{202} with Seven Heptagon Rings

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ABSTRACT

In this proposal, some examples of nonclassical fullerenes with seven heptagon rings are presented. The first one, a fullerene with 192 carbons, seven heptagons, 19 pentagons, and 72 hexagons, is considered. The other fullerene with seven heptagon rings is constituted by 202 carbons. Application GeoGebra, and software CaGe are utilized to generate representations of considered molecules. Schlegel diagrams are also provided. Our goal is to look for structural patterns in this type of fullerenes.

Keywords: nonclassical fullerenes, Isolated pentagon Rule, CaGe, GeoGebra

1 INTRODUCTION

The first example that we consider of a nonclassical fullerene [1], [2] contains 192 carbons. There are 7 heptagons, the number of hexagons is 72, and finally, we have 19 pentagons. One of the seven heptagons is surrounded by 6 hexagons, and just one pentagon. Then, three heptagonal rings are surrounded by two pentagons, and five hexagons. Furthermore, three heptagons are surrounded by three pentagons, and four hexagons.

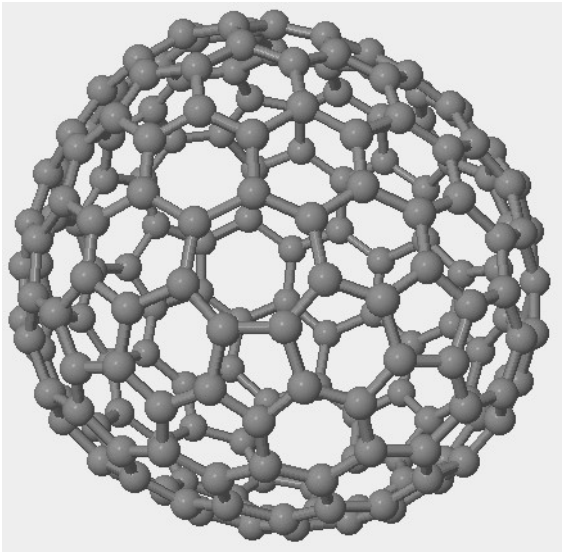

Figure 1: Fullerene with 192 carbons.

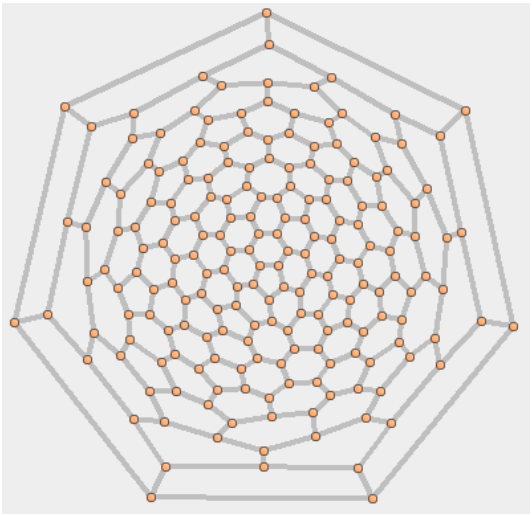

Figure 2: Schlegel diagram of fullerene C_{192}.

One the other hand, to get the second fullerene, we consider a fullerene with 204 carbons, that is formed by six

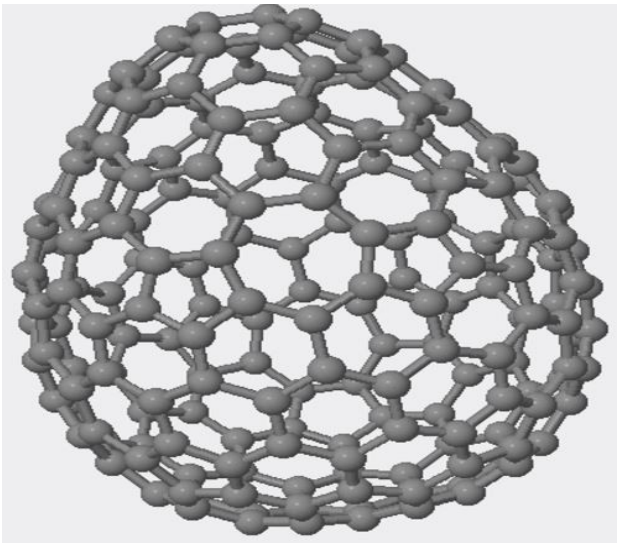

Figure 3: Fullerene with 204 carbons.

heptagons, 80 hexagons, and 18 pentagons.

2 CALCULATIONS

The fullerene with 204 carbons shown in Figures 3 and 4, is going to be slightly modified. Close to the bottom of Figure 4, appears one hexagon surrounded by three pentagons, and three more hexagons. At Figure 5, is displayed the central hexagon, and the three pentagons. Carbons denoted by E, and F will be suppressed, and pentagon with vertices E, F, J, H, and G, will be merged with hexagon such that its vertices are E, F, D, B, A, and C, to generate a heptagon with vertices G, H, J, D, B, A, and C, that is shown in Figure 5. With this process, two new pentagons are built, but one of the original pentagons, is absorbed by the new heptagon. Similarly, when 2 carbons are deleted, two hexagons are transformed into two pentagons, and one more hexagon, will be included in the heptagon number seven. Therefore, we obtain a fullerene with 202 carbons, 80 minus three, equal to 77 hexagons, 18 plus one, equal to 19 pentagons, and 7 heptagons. Formulas found in [3] are given by

$$5\,p + 6\,h + 7\,s = 3\,n$$

$$2\,p + 2\,h + 2\,s = n + 4$$

where n is the number of carbons of considered fullerene, p is the number of pentagon rings, h is the number of hexagonal rings, and s is the number of heptagon rings. If $n = 202$, and $s = 7$ are substituted

$$5\,p + 6\,h = 606 - 49 = 557$$

$$2\,p + 2\,h = 206 - 14 = 192$$

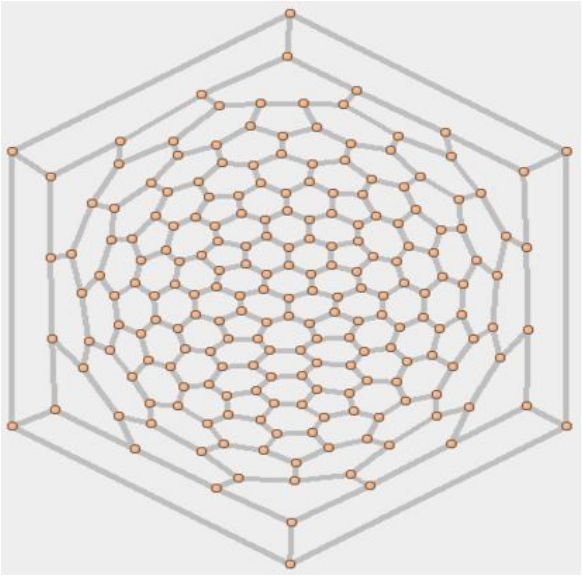

Figure 4: Schlegel diagram of C_{204}.

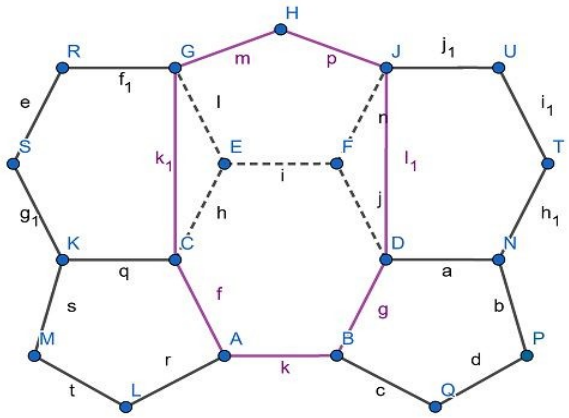

Figure 5: New heptagon obtained from one pentagon and one hexagon. Also, two hexagons become pentagons.

then, $p = 19$, and $h = 77$ are actually obtained as solutions of the system of two equations.

3 DISCUSSION

Two types of nonclassical fullerenes have been presented: the first one with 192 carbons, and 72 hexagons. The second fullerene has 202 carbons, and 77 hexagons. Both fullerenes has 19 pentagons. Fullerene C_{192} satisfies the isolated pentagon rule IPR. That is, there are no pentagon located next to another pentagon. Examples of fullerenes with 130, and 134 carbons, containg also 7 heptagon rings are found in [4]. Cage software [5] has been used to generate the fullerenes, but Figure 5 was obtained with GeoGebra.

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