Nonclassical Fullerenes C_{60} and C_{66} with Five Heptagon Rings

Francisco J. Sánchez-Bernabe*

*Universidad Autónoma Metropolitana Iztapalapa
San Rafael Atlixco 186, Ciudad de México 09310, Mexico, fjsb@xanum.uam.mx

ABSTRACT

In this paper, a couple of nonclassical fullerenes with five heptagon rings are presented. The first one, a fullerene with 60 carbons, five heptagons, 17 pentagons, and 10 hexagons, is considered. The other fullerene with five heptagon rings is constituted by 66 carbons. Software CaGe is utilized to generate representations of considered molecules. Schlegel diagrams are also provided. Our goal is to look for patterns in the structural diagrams of fullerenes with five heptagon rings.

Keywords: nonclassical fullerenes, Isolated pentagon Rule, CaGe

1 INTRODUCTION

The first example that we consider of a nonclassical fullerene [1], [2] contains 60 carbons. There are five heptagons, the number of hexagons is 10, and finally, we have 17 pentagons. One of the five heptagons is surrounded by five pentagons, and two hexagons. Then, a couple of heptagonal rings are placed next to each other, and sharing two pentagons. The additional rings that surrounds each of these couple of the heptagons, are two hexagons, and two pentagons.

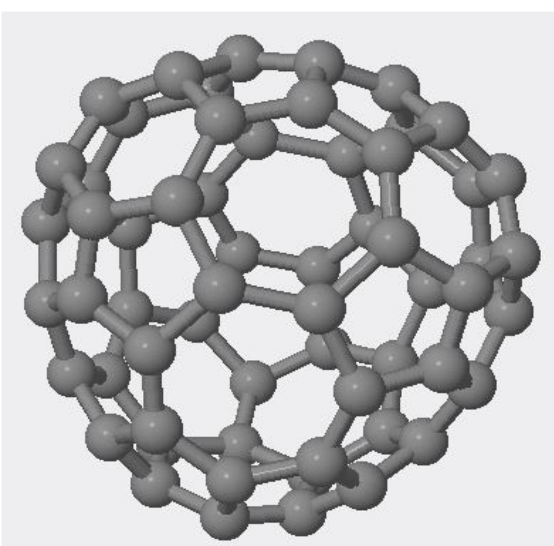

Figure 1: Fullerene with 60 carbons.

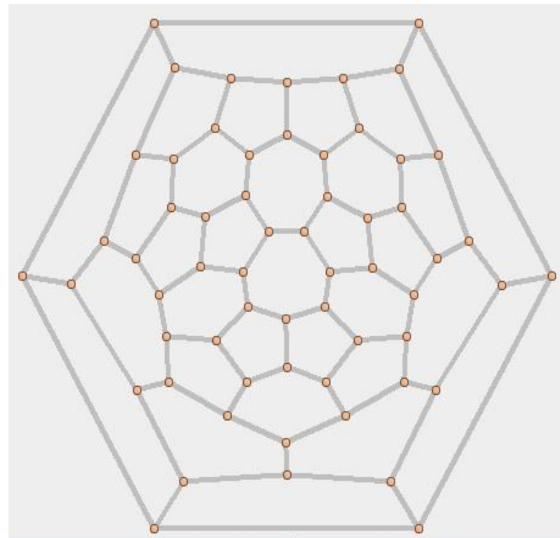

Figure 2: Schlegel diagram of fullerene C_{60}.

Finally, two heptagons are surrounded by three hexagons, and four pentagons.

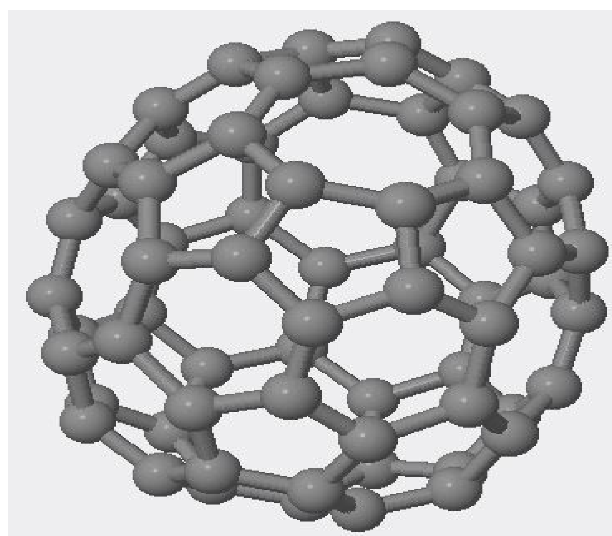

Figure 3: Fullerene with 66 carbons.

On the other hand, the other fullerene has 66 carbons.

2 CALCULATIONS

If n is the number of carbons of considered fullerene, formulas found in [3] are given by

$$5p + 6h + 7s = 3n$$
$$2p + 2h + 2s = n + 4$$

where p is the number of pentagon rings, h is the number of hexagonal rings, and s is the number of heptagon rings. If $n = 60$, and $s = 5$ are substituted

$$5p + 6h = 180 - 35 = 145$$
$$2p + 2h = 64 - 10 = 54$$

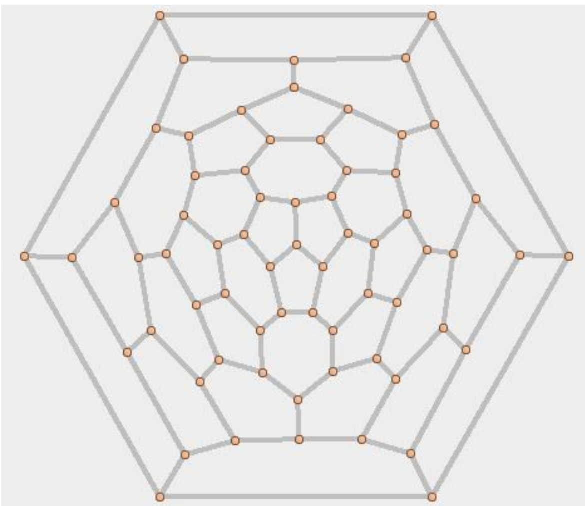

Figure 4: Schlegel diagram of C_{66}.

then, $p = 17$, and $h = 10$ are actually obtained as solutions of the system of two equations.

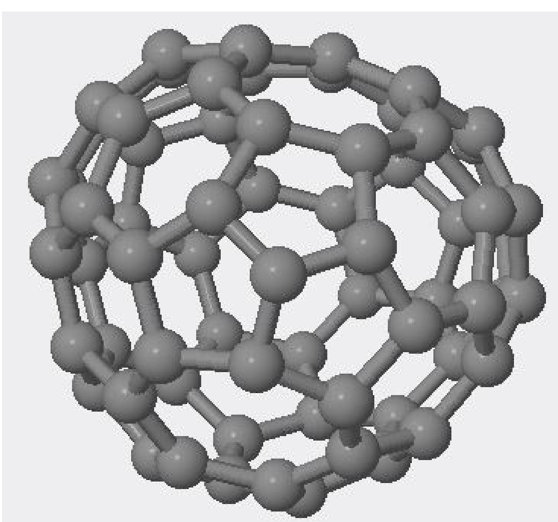

Figure 5: Another view of fullerene C_{66}.

Similarly, if $n = 66$, and $s = 5$ are substituted into the same system of equations

$$5p + 6h = 198 - 35 = 163$$
$$2p + 2h = 70 - 10 = 60$$

we obtain $p = 17$, and $h = 13$.

3 DISCUSSION

Two types of nonclassical fullerenes have been presented: the first one with 60 carbons, and 10 hexagons. The second fullerene has 66 carbons, and 13 hexagons. Both fullerenes has 17 pentagons. Neither fullerene C_{60} or C_{66} satisfies the isolated pentagon rule IPR. That is, there exists at least one pentagon located next to another pentagon. Examples of fullerenes with 2, 3, 4, and 6 heptagon rings are found in [4]. Cage software [5] has been used to generate the fullerenes.

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