

On A Fullerene with 458 Carbons

Containing 8 heptagonal rings

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Abstract—A Fullerene with pentagons, hexagons, and heptagons is considered. The number of carbons is 458. It contains 8 heptagonal rings, 21 pentagons, and 212 hexagons.

Keywords—component; fullerene; heptagon; pentagon adjacency penalty rule; fullerene with many carbons

I. INTRODUCTION

According to Fowler and Manolopoulos [1], classical fullerenes are those carbon cage molecules with exactly 12 pentagons and $n/2 - 10$ hexagons. All classical fullerenes satisfy the so called isolated pentagon rule IPR, Kroto [2]. On the other hand, nonclassical fullerenes are those carbon cage molecules, such that one or more squares or heptagons, appears. In this last case, sometimes pentagon-pentagon adjacencies are observed, and the most stable structure are related with the least pentagon-pentagon adjacencies, which is known as the pentagon adjacency penalty rule PAPR, Campbell *et al* [3].

Work has been done to study nonclassical fullerenes; for example, 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] studied the isomers of fullerene C_{26} composed of square, pentagonal, hexagonal, and heptagonal faces. Also, Tchoffo *et al* [6] present fullerenes with square and octagonal faces. 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. Finally, D.-L. Chen *et al* [8] study fullerene C_{58} .

II. BACKGROUND

Previously, it was presented a study, Sánchez-Bernabe *et al* [9] considering the type of neighbours that an heptagonal ring may present: the first example contains 68 carbons with two heptagonal rings, and also 14 pentagons, completed with 20 hexagons.

The second example has 80 carbons, with three heptagons, 15 pentagons, and 24 hexagons. The next example of nonclassical fullerene contains 82 carbons with four hexagonal rings, 16 hexagons, and 23 hexagons. The fourth example has 76 carbons with six heptagons, 18 pentagons, and 16 hexagons. The next example of fullerene contains 64 carbons with five heptagonal rings, 17 pentagons, and 12 hexagons. Finally, it was considered a fullerene with 42 carbons, two heptagonal rings, 14 pentagons, and 7 hexagons.

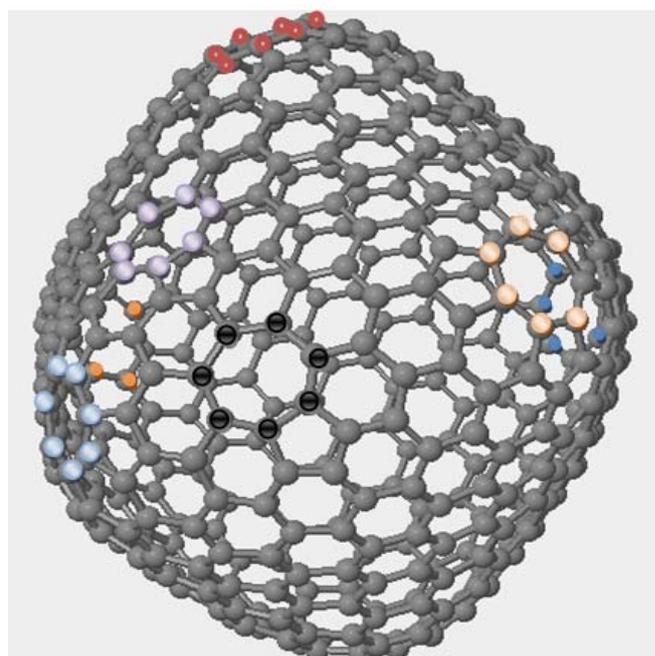


FIGURE 1. FRONT VIEW OF THE 458 CARBONS FULLERENE

III. CALCULATIONS

We present a fullerene with 458 carbons. In FIGURE. 1, we observe three close heptagons, with light blue, black and the third heptagon above the two previous heptagons. Two heptagons, have a peculiar feature: they are surrounded by six hexagons and only one pentagon; the other heptagon has contact with four hexagons and three pentagons. At the "north pole" of the molecule, we have a heptagonal ring surrounded by four hexagons and three pentagons. At the left side of the fullerene we observe an orange heptagonal ring surrounded by four hexagons and three pentagons. Next, at the right side, we have a heptagon finally, we observed four carbons of another heptagonal ring located at the rear of the molecule; it is surrounded by four hexagons and three pentagons. Therefore, we have seven heptagonal rings in FIGURE. 1.

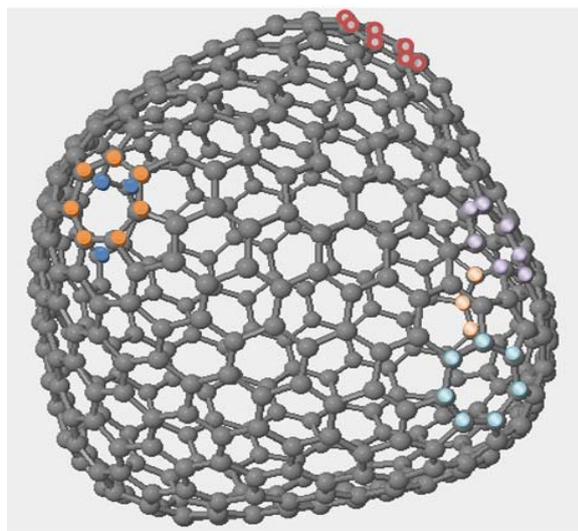


FIGURE II. VIEW FROM LEFT SIDE OF THE FULLERENE

In FIGURE II we observe again the pink heptagon, and one of the heptagons located at the front of the molecule, this heptagon is surrounded by four hexagons and three pentagons. Next, in FIGURE. III, we observe the heptagon number 8 at the bottom, it is surrounded by four pentagons and three hexagons.

We have obtained the graphs of our results by running the V0.3 version of (Carbon Generator) CaGe software, [10].

IV. CONCLUSIONS

We present a 458 carbons fullerenes, 8 heptagons, 21 pentagons, and 212 hexagons. This number is higher than the molecules we have considered in previous papers. We are working on a procedure to increase the number of molecules.

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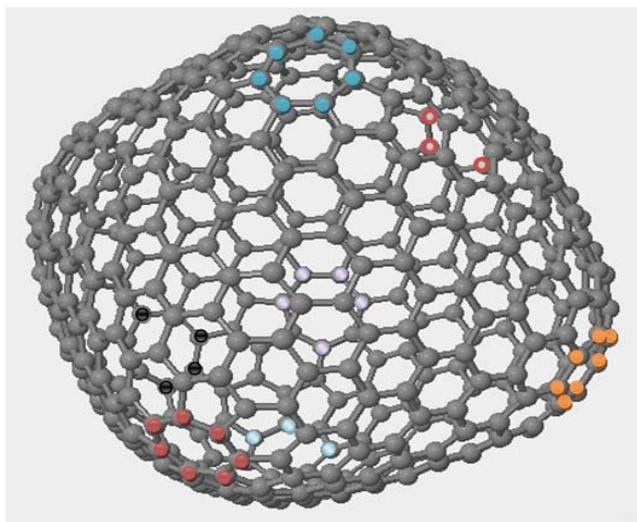


FIGURE III. BACK VIEW OF THE 458 CARBONS FULLERENE

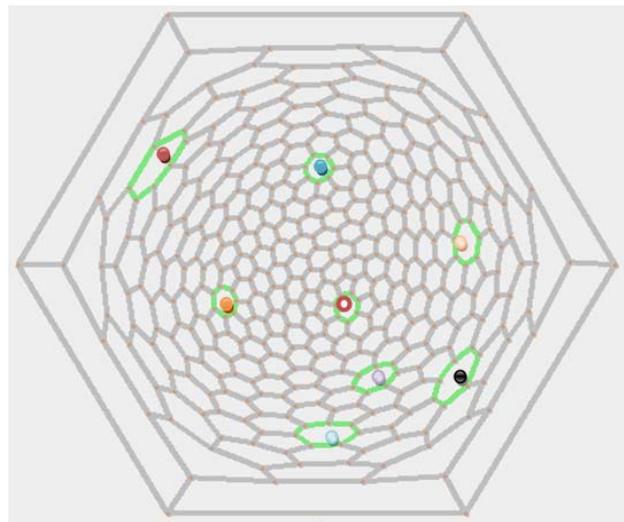


FIGURE IV. SCHLEGEL DIAGRAM OF THE FULLERENE

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