Nonclassical Fullerenes with Cubic and Octahedral Structure

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ABSTRACT

Classical fullerenes are molecules consisting of pentagons and hexagons. As a matter of fact, each classical fullerene contains exactly 12 pentagons as a consequence of Euler's Theorem. On the other hand, nonclassical fullerenes contains also, square, heptagonal, or octagonal faces. Several works have considered fullerenes with heptagonal rings; for instance in [1]. Another fields where nonclassical fullerenes appear are shown in [2], [3], [4], [5], and [6].

Keywords: nonclassical fullerenes, Euler's Theorem, Isolated pentagon Rule, Schlegel diagram

1 CALCULATIONS

The first example that we consider of a nonclassical fullerene contains 128 carbons. There are 12 heptagons. The number of hexagons is 30, and finally, we have 12 pentagons. As can be observed from Figure 1, each *face* of this cubic structure is formed by 4 heptagons, separated by 5 hexagons, and 4 pentagons, located at each of its corners.

The corresponding Schlegel Diagram of this Fullerene with 128 carbons is shown in Figure 2. At the central part of this Diagram, we appreciate one hexagon with a couple of this type of polygons to the left, and to the right of the first hexagon. There is one heptagon at the top of the central hexagon, and another heptagon at the bottom. A couple of pentagons touch the heptagon located at the top, and another couple of pentagons, touch the heptagon at the bottom.

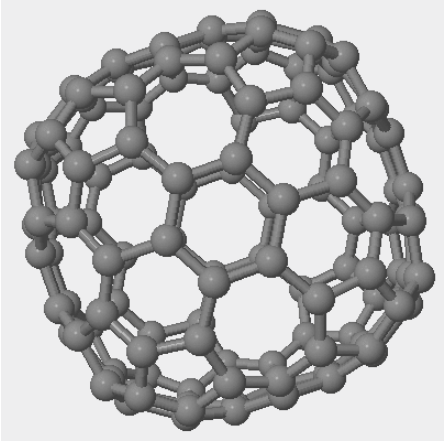

Figure 1: Fullerene with 128 carbons.

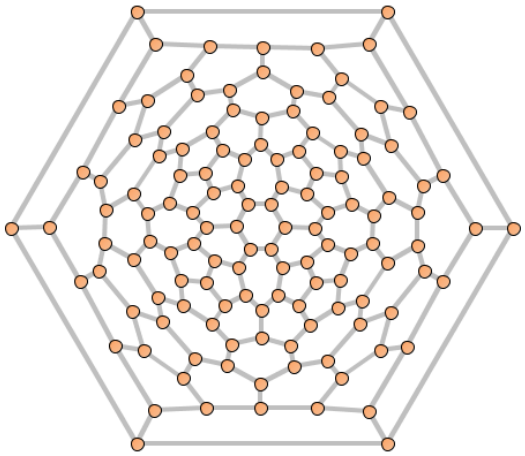

Figure 2: Schlegel Diagram of Fullerene C_{128}.

The fullerene with octahedral structure is formed by 132 carbons, is shown in Figure 3. In this case, there are two types of *faces*. One of them, that can be observed at the central part of molecule of Figure 3, has a central hexagon surrounded by 3 heptagons, and 3 pentagons. Two pentagons, next to each other, separate this face to the other 3 faces of the same structure.

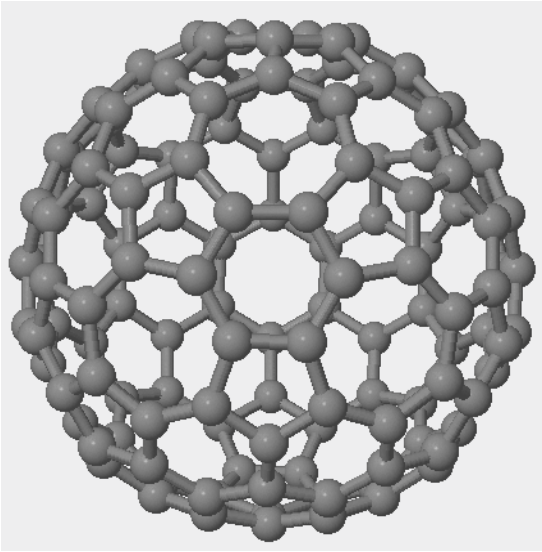

Figure 3: Fullerene with 132 carbons.

The other type of face is more conventional, because contains one hexagon, with 6 neighbours, that are also hexagons. This pattern, is appreciated at the central part of Schlegel Diagram of Figure 3. Thus, this fullerene has 8 faces, 4 of one type, and the other 4, of the other type. We have used Cage [8] for processing our graphs.

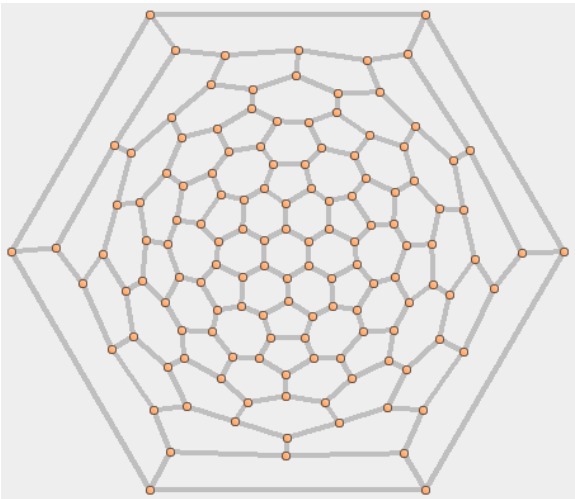

Figure 4: Schlegel Diagram of Fullerene C_{132}.

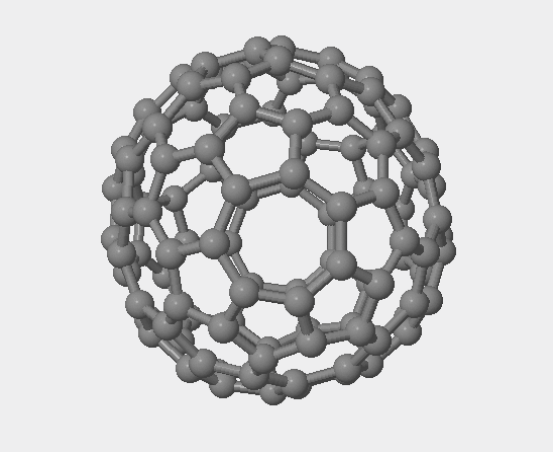

Figure 5: Fullerene with 112 carbons.

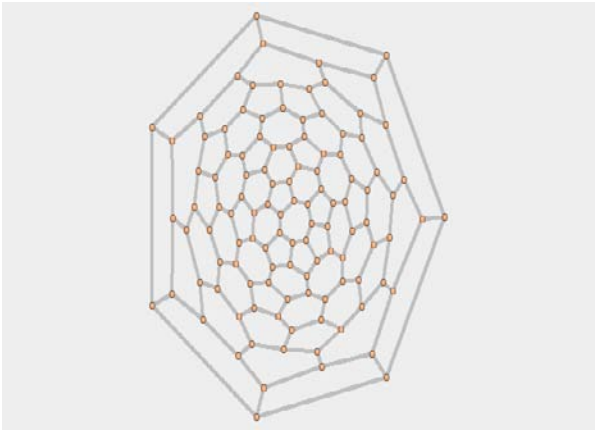

Figure 6: Schlegel Diagram of Fullerene C_{112}.

2 DISCUSSION

Two types of nonclassical fullerenes have been presented: the first one with 128 carbons, with a cubic structure. Meanwhile, the second example, with 132 carbons, has octahedral structure. We also present a fullerene with 112 carbons. Fullerenes are important on diverse applications: toxic gas sensors, fabrication of flat panel displays, conducting paints.

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