Two Examples of Nonclassical Fullerenes with Dodecahedral 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

1 CALCULATIONS

The first example that we consider of a nonclassical fullerene contains 420 carbons. There are 60 heptagons. The number of hexagons is 80, and finally, we have 72 pentagons. As can be observed from Figure 1, each *face* of this structure is formed by one pentagon at the center, surrounded by 5 heptagons, and then, there are 5 pentagons at the corners.

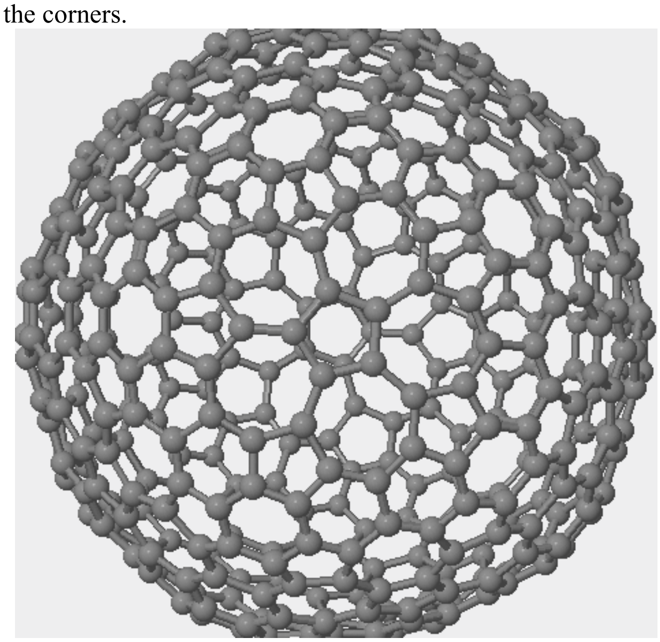

Figure 1: Fullerene with 420 carbons.

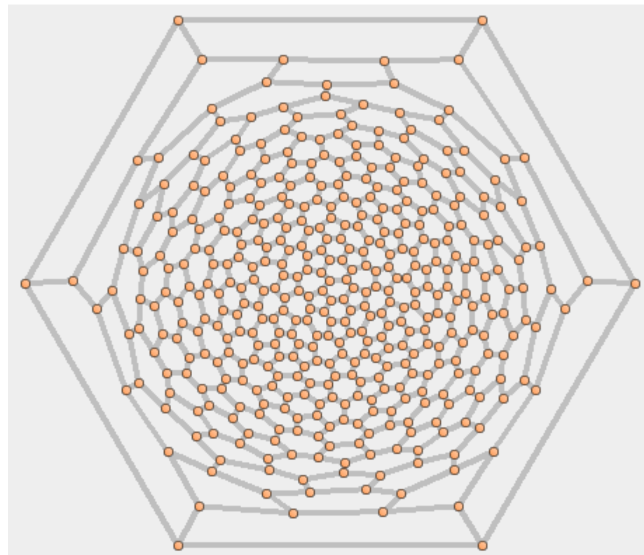

Figure 2: Schlegel diagram of first example fullerene.

The face is completed by 5 hexagons at outer corners. Each of these hexagons is separated a couple of hexagons, forming a ring of 15 hexagons.

We can count the number of edges of this fullerene in the following way. We have 5 edges for each pentagon in the center, plus 5 more edges joining this pentagon with the surrounded pentagons. Each of this 5 pentagons, have two edges which meet the radial edges, giving 5 times 2, equal to 10 more edges. So, up to now, we have 5 plus 5 plus 10, equal to 20 inner edges. Since we have 12 faces, we obtain 12 times 20. Equal to 240 inner edges.

Now, the ring of 15 hexagons that separate each face have edges in common with these faces. In order no to count the edges more than once. Let us consider the 20 hexagons that determine the corners of the faces. There are 6 edges for each of these hexagons, and there are 4 additional edges of each of the 3 hexagons connected with of the 20 hexagon at the corners. So, we have 6 plus 12 edges equal to 18 edges for each of the 20 corners. This means 360 edges. But there are one more edge separating this collection of 20 structures with 4 hexagons. Since, the 20 corners are joined by 30 *edges* form by 2 hexagons, we have 30 more edges. Therefore, we have a total number of 240 plus 360 plus 30, equal to E = 630 edges.

Now, the number of faces F is equal to 60 heptagons plus 80 hexagons plus 72 pentagons, equal to F = 212

Since, the number of vertex V is equal to 420, we know by Euler's formula that

$$630 + 2 = E + 2 = V + F = 420 + 212 = 632$$

In our second example with 200 carbons, each *face* of this structure is formed by one pentagon, surrounded by 5 heptagons, and 5 squares at the corners. Each of the 12 faces are separated by a ring of 10 heptagons.

The number of edges is counted in the following way. We have 5 edges for each pentagon, then another 5 edges that connect the pentagon with each square. Then, each of these 5 squares, have 2 edges contained in each face, giving 10 more edges. So, up to now, we have 5 plus 5 plus 10, equal to 20 edges. Additionally, at the corner of each face, meet 3 heptagons with one edge in common for each couple of faces. This means that we have to count only one of these edges to each face, giving 5 more edges to each face. Therefore, we have 20 plus 5, equal to 25 edges per each face. Summarizing, we have 25 times 12 faces, which give us E = 300 edges. On the other hand, we have 12 pentagons plus 30 squares, plus 60 heptagons, so the total number of faces F is equal to 102. Since, the number of vertex V is equal to 200, by Euler's formula, we have that

$$300 + 2 = E + 2 = V + F = 200 + 102 = 302$$

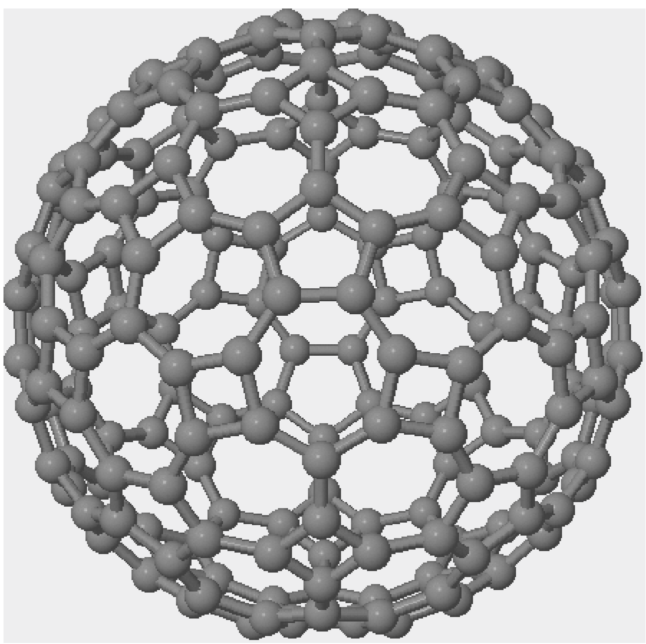

Figure 3: Fullerene with 200 carbons.

2 DISCUSSION

Two types of nonclassical fullerenes have been shown: the first one with 420 carbons, the second, with

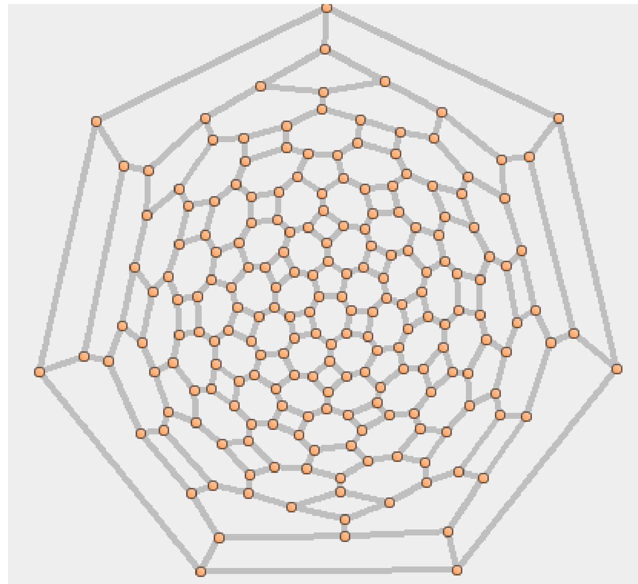

Figure 4: Schlegel diagram of fullerene C_{200} .

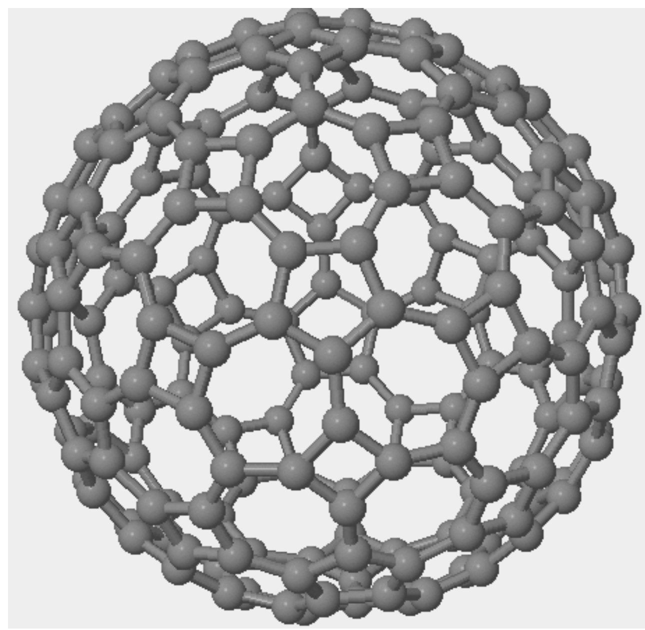

Figure 5: Another view of fullerene with 200 carbons.

200 carbons. The first fullerene is constituted by 60 heptagons, 80 hexagons, and 72 pentagons. The molecule with 200 carbons is formed by 60 heptagons, 12 pentagons, and 30 squares. Surprisingly, this last fullerene contains no hexagon. A more recent work [10] also have used Cage software to generate the fullerenes, they observe that the pentagons and hexagons involved are not regular. Fullerenes are important on diverse applications: toxic gas sensors, fabrication of flat panel displays, and conducting paints, between many others

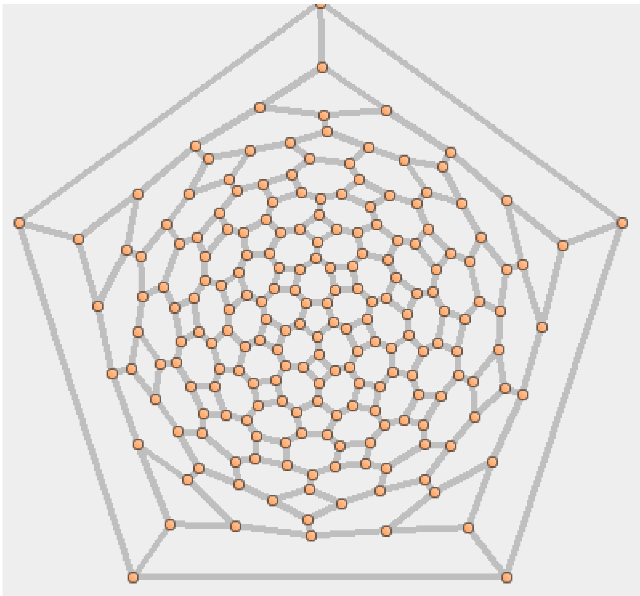

Figure 6: Another Schlegel diagram of fullerene C_{200}.

REFERENCES

[1] A. Ayuela, P.W.Fowler,D.Mitchell,R Schmidt,G.Seiftert,and F.Zerbetto, “C_{62}: Theroretical Evidence for a Nonclassical Fullerene with a heptagon ring” in J. Phys. Chem., vol 100 pp 15634-36, 1996.

[2] S. Gaito, L Colombo, and G. Benedek , “A Theroretical study of the smallest tetrahedral carbon schwarzites", in Europhysics Letters, vol. 44. (44) 1998.

[3] F. Beuerle, C. Herrmann, A. C. Whalley, C. Valente, A. Gamburd, M. A.Ratnerl, and J. F. Stodard, “Optical and Vibrational Properties of Toroidal Carbon Nanotubes", in Chem. Eur. J., vol. 17, pp. 3868-3875, 2011.

[4] C. Chuang, Yuan-Chia Fan, and Bih-Yaw Chin, “Comments on Structural Types of Toroidal Carbon Nanotubes” in arXiv: 1212.4567 2012

[5] C. Chuang, Yuan-Chia Fan, and Bih-Yaw Jin, “Generalized Classification Scheme of Toroidal and Helical Carbon Nanotubes”, in J. Chem. Inf. Model., vol. 49, No. 2, pp. 361-368, 2009

[6] F. J. Sánchez-Bernabe and J. Salcedo, “Construction of a Fullerene with 570 carbons: Containing 7 Heptagonal Rings”, 5th Annual Int Conf. on Comp. Math, Comp. Geo. & Statistics, 2016

[7] H. W. Kroto, J. R. Heath, S.C. O'Brien, R.F. Curl, and R.E. Smalley, “C_{60}: Buckminsterfullerene ” in Nature. Vol. 318, pp. 162-163, 1985

[8] G. Brinkmann, O. Delgado, S. Friedrichs, A. Lisken, A. Peters and N.V. Cleemput, CaGe - a Virtual Environment for Studying Some Special Classes of Plane Graphs-an update, MATCH Commun. Math. Comp. Chem. 63(3): 533-552, 2010

[9] Fleischner,H, “Reducing an arbitrary fullerene to the dodecahedron”, in Discrete Mathematics 340 (2017) Issue 11 2714-2722

[10] Andova V and Kardos F, “Mathematical aspects of fullerenes”, in Ars mathematica contemporanea 11, (2016) 353-379