F. J. Sánchez-Bernabe
Department of Mathematics Metropolitan Autonomous University
e-mail: fjsb@xanum.uam.mx

CONSTRUCTION OF CLASSICAL AND NONCLASSICAL FULLERENES WITH TETRAHEDRAL STRUCTURE

Classical fullerenes are molecules with pentagons and hexagons. On the other hand, nonclassical fullerenes contain also, squared, heptagonal, or octagonal faces.

Calculations

The first example that we consider is a classical fullerene that contains 56 carbons. We observe in Figure 1, that at the upper part of the molecule, there are two pentagons next to each (actually there is another one behind them). This means that our fullerene, does not satisfy the Isolated pentagon Rule, IPR.

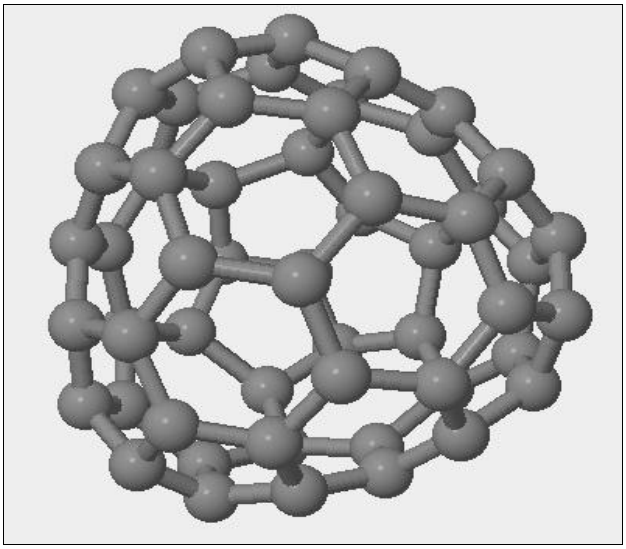

Figure 1. – Classical fullerene with 56 carbons

We observe in Figure 2 three pentagons located next to each other.

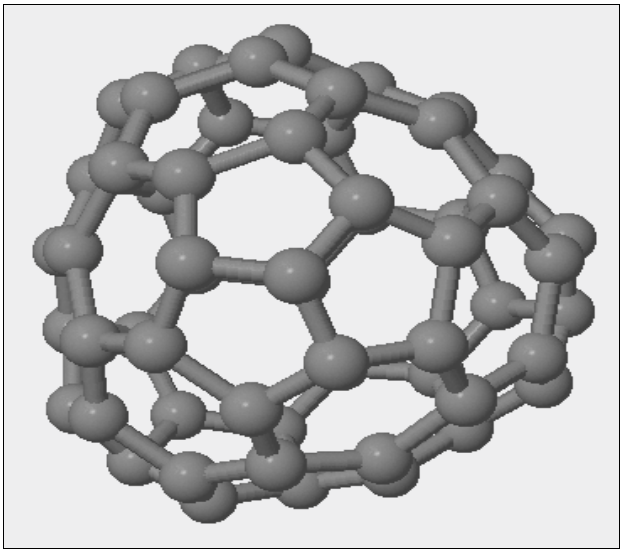

Figure 2. – View from the top of fullerene C_{56}

Schlegel diagram of fullerene C_{56} showing one face composed by three hexagons, that is located above the equator of the graph, and another face, below that horizontal zone.

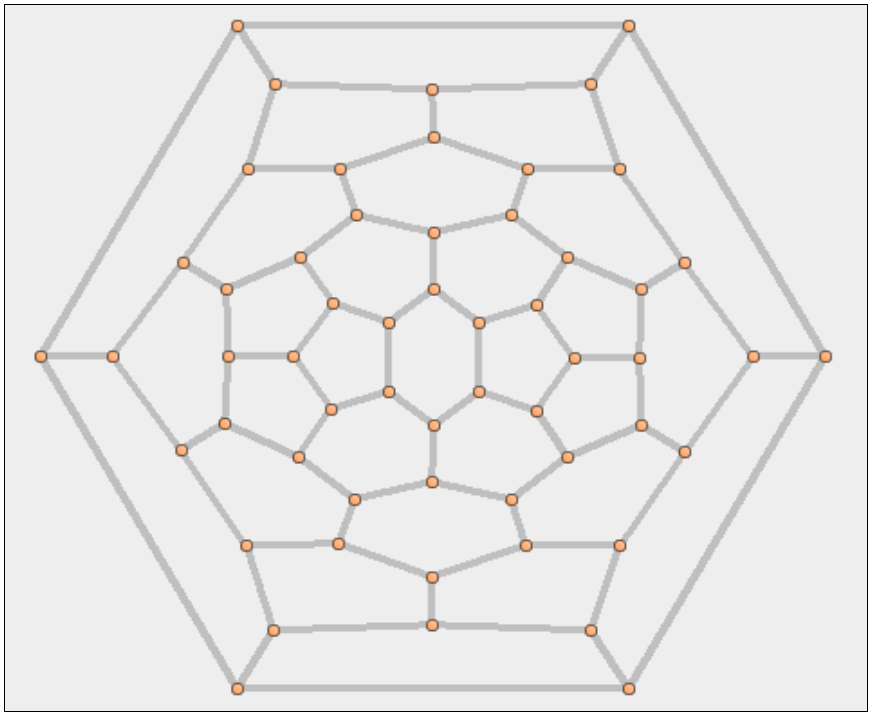

Figure 3. – Schlegel diagram of fullerene C_{56} showing two of the four faces with three hexagons

At our Schlegel diagram, we observe four groups with 3 hexagons, each of them. Next, w add, six hexagons that separate a couple of three pentagons, and two faces with three hexagons. Thus, 4 times 3 plus 6 is equal to 18 hexagons, and 12 pentagons.

Our next molecule contains heptagons. Thus, it is an example of a nonclassical fullerene. We have 64 carbons, 12 pentagons, 10 hexagons, and 12 squares.

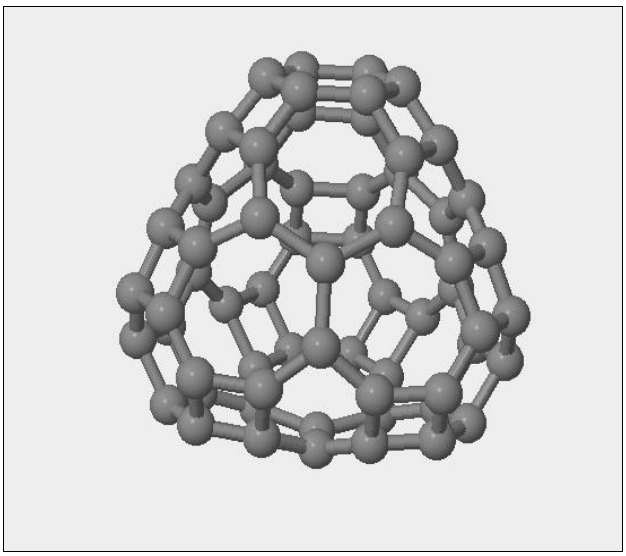

Figure 4. – One of the four faces of C_{64} is constituted by four heptagons

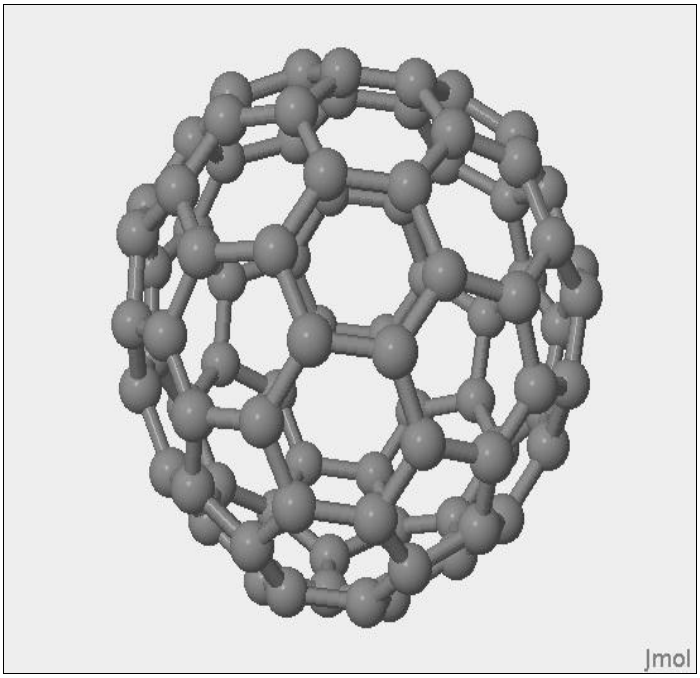

Figure 5. – Classical fullerene C_{84} with tetrahedral symmetry

In order to obtain the nonclassical fullerene C_{64}, we consider the C_{84} classical isomer with tetrahedral structure, and we replace the seven hexagons located next to each other (that form a face) by three heptagons. The original face has 12 inner carbons, and the new face contains 10 inner carbons. Therefore, after this first step, a nonclassical fullerene with 82 carbons is generated, which is shown in Figure 6.

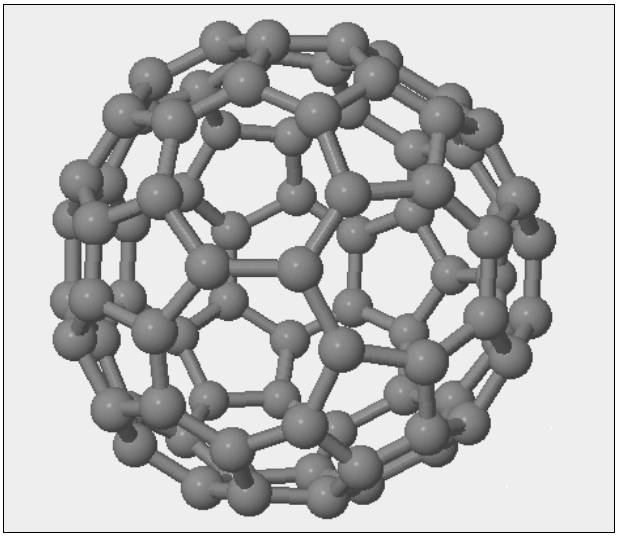

Figure 6. – Nonclassical fullerene with 82 carbons

Moreover, on Figure 6, we can observe that between the new face and the original ones, a pentagon takes the place of a previous hexagon. After we replace another face of seven hexagons by three heptagons we obtain a nonclassical fullerene with 78 carbons, see Figure 7.

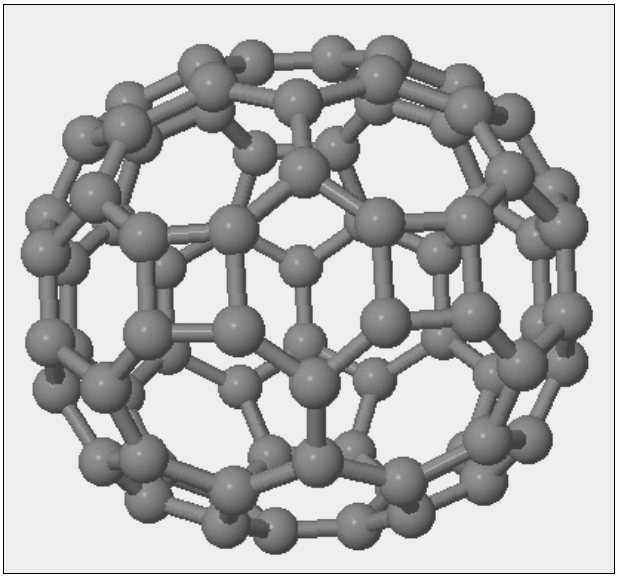

Figure 7. – Nonclassical fullerene with 78 carbons

Meanwhile, on Schlegel diagram of Figure 8, we have a couple of squares.

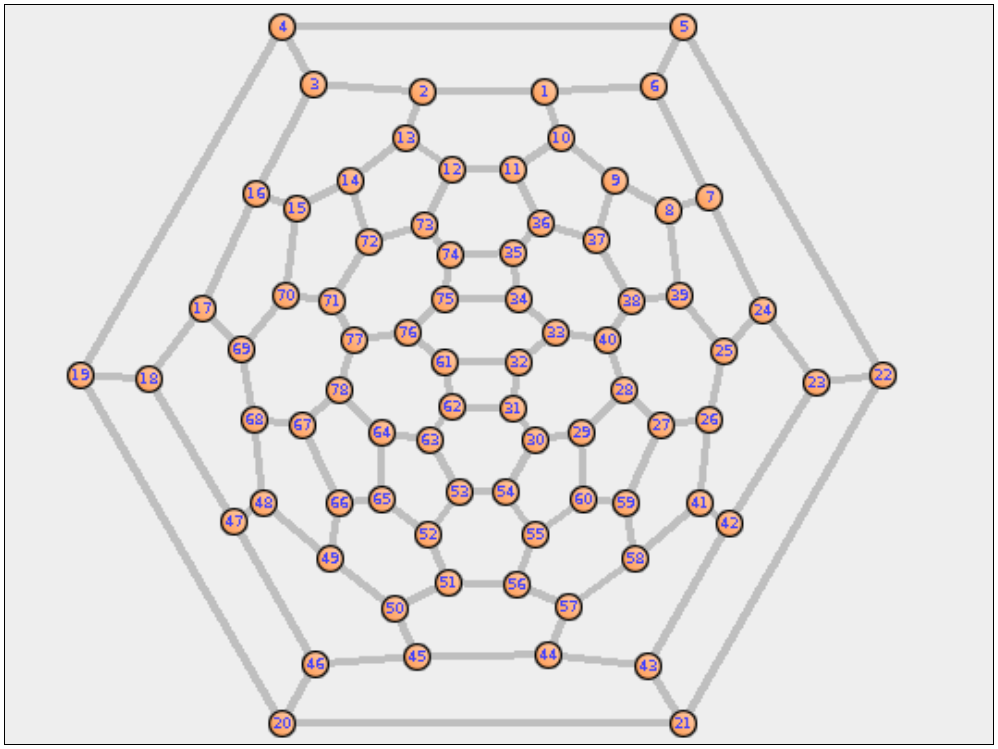

Figure 8. – Schlegel diagram of nonclassical fullerene with 78 carbons

Next, we repeat this procedure for the third time to obtain a nonclassical fullerene with 72 carbons, which is shown in Figure 9. Finally, after a last iteration, we have the nonclassical fullerene with 64 carbons of Figure 4.

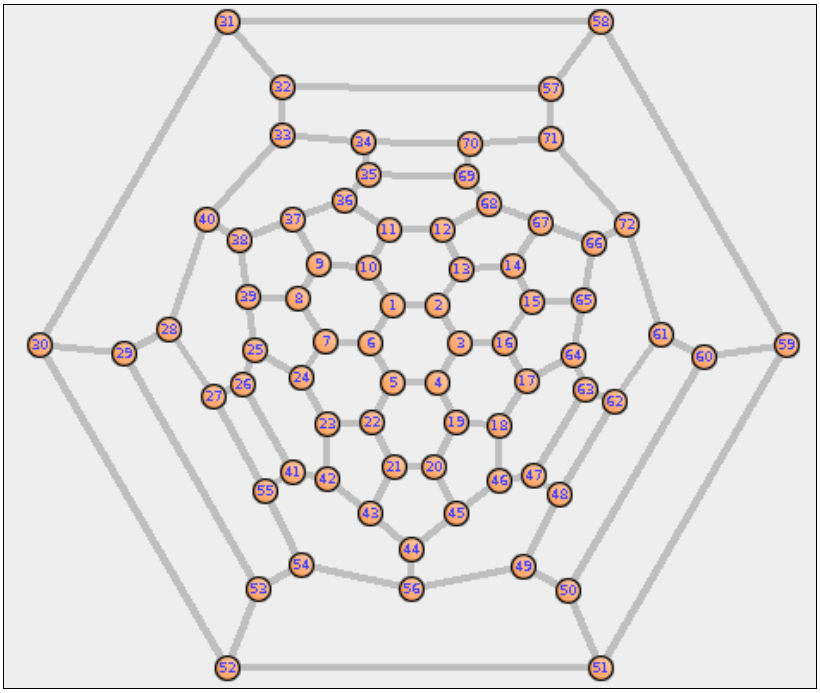

Figure 9. – Schlegel diagram of nonclassical fullerene with 72 carbons

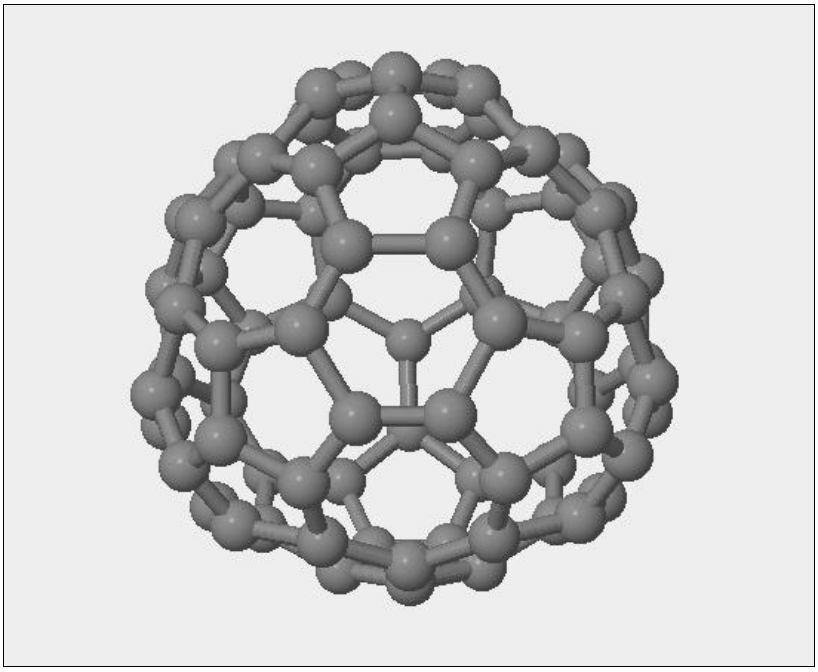

Figure 10. – Nonclassical fullerene with 76 carbons

In our previous construction, the faces formed by three heptagons, have hexagons as vertexes, and between two hexagons there is a boundary filled out with one hexagon and two squares. But, if this boundary consists of four pentagons, instead of squares and the hexagon, for each one of the six boundaries, we have two additional carbons, which give 12 more carbons. Therefore, we obtain a new nonclassical fullerene with 64 plus 12 equal to 76 carbons, which is shown in Fig. 10.

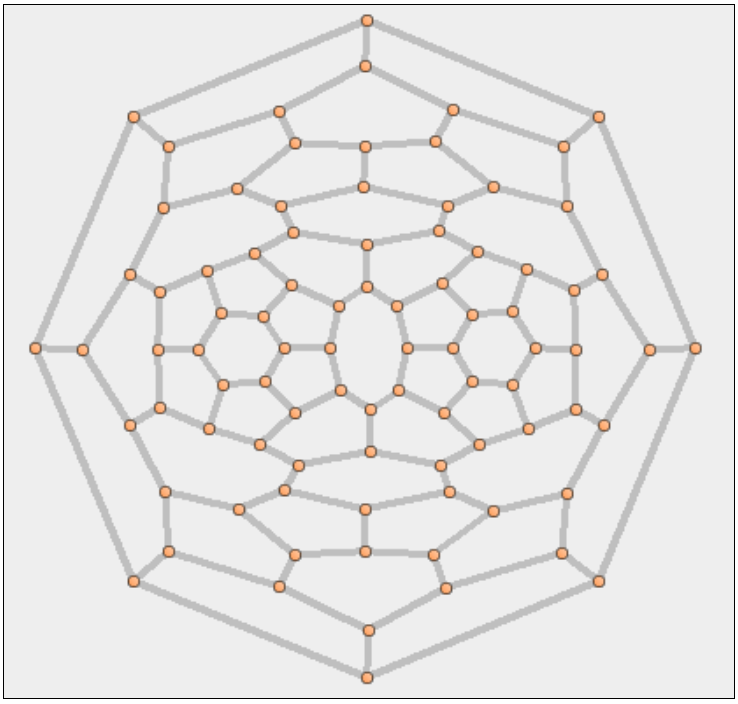

Figure 11. – Nonclassical fullerene with 88 carbons, containing 6 octagons

Now, we consider a fullerene with 88 carbons, containing 6 octagons

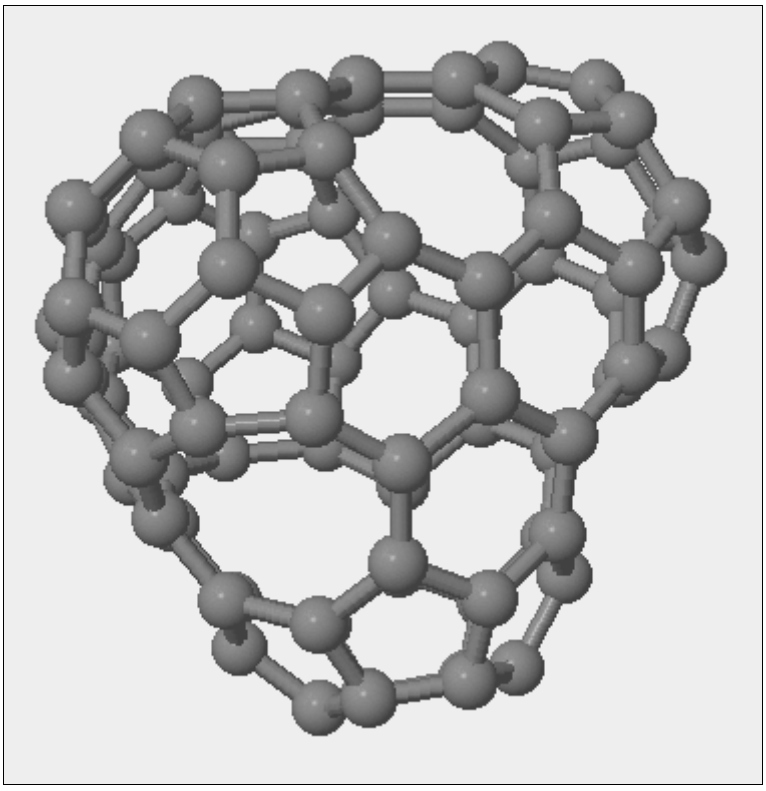

Figure 12. – One of the four corners of a nonclassical fullerene with 88 carbons

We observe four corners constituted by one hexagon surrounded by six hexagons.

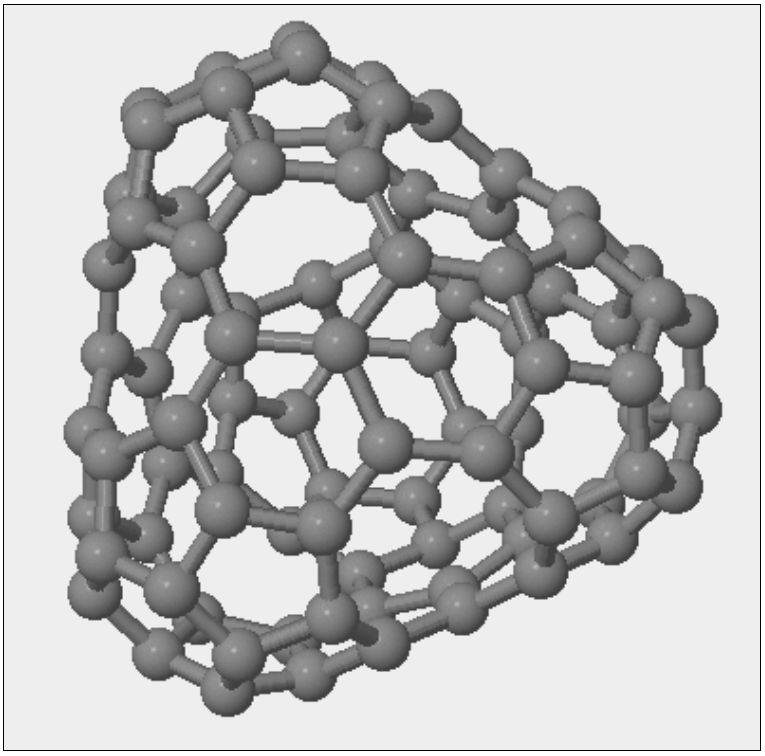

Figure 13. – One of the four faces integrated by three hexagons

Then, we have 12 hexagons coming from the four faces, plus 4 more hexagons from the corners, giving a total of 16 hexagons. Now, we take into account 24 pentagons from the four corners, and 6 octagons.

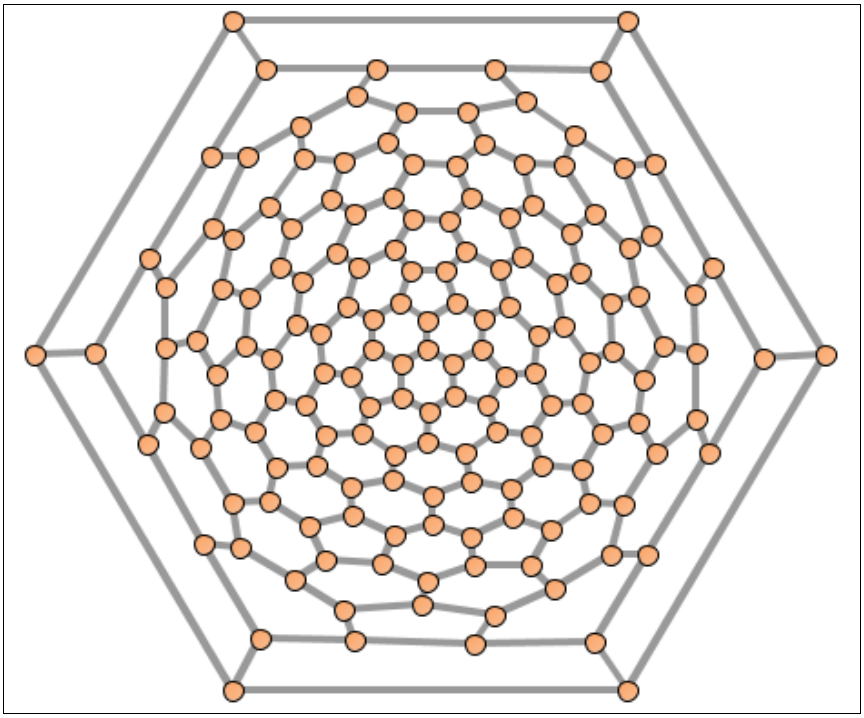

Figure 14. – Schlegel diagram of a classical fullerene with 160 carbons

In order to generate another nonclassical fullerene, we consider the C_{160} classical isomer with tetrahedral structure, with Schlegel diagram shown on Figure 14 and, we replace

the three hexagons located next to each other (that form a face) by three heptagons, see Figure 15

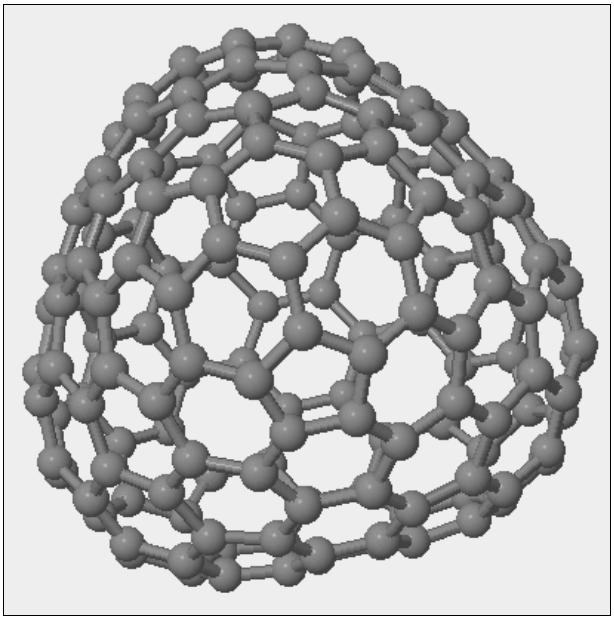

Figure 15. – Intermediate step to obtain a152 carbons fullerene from C_{160}

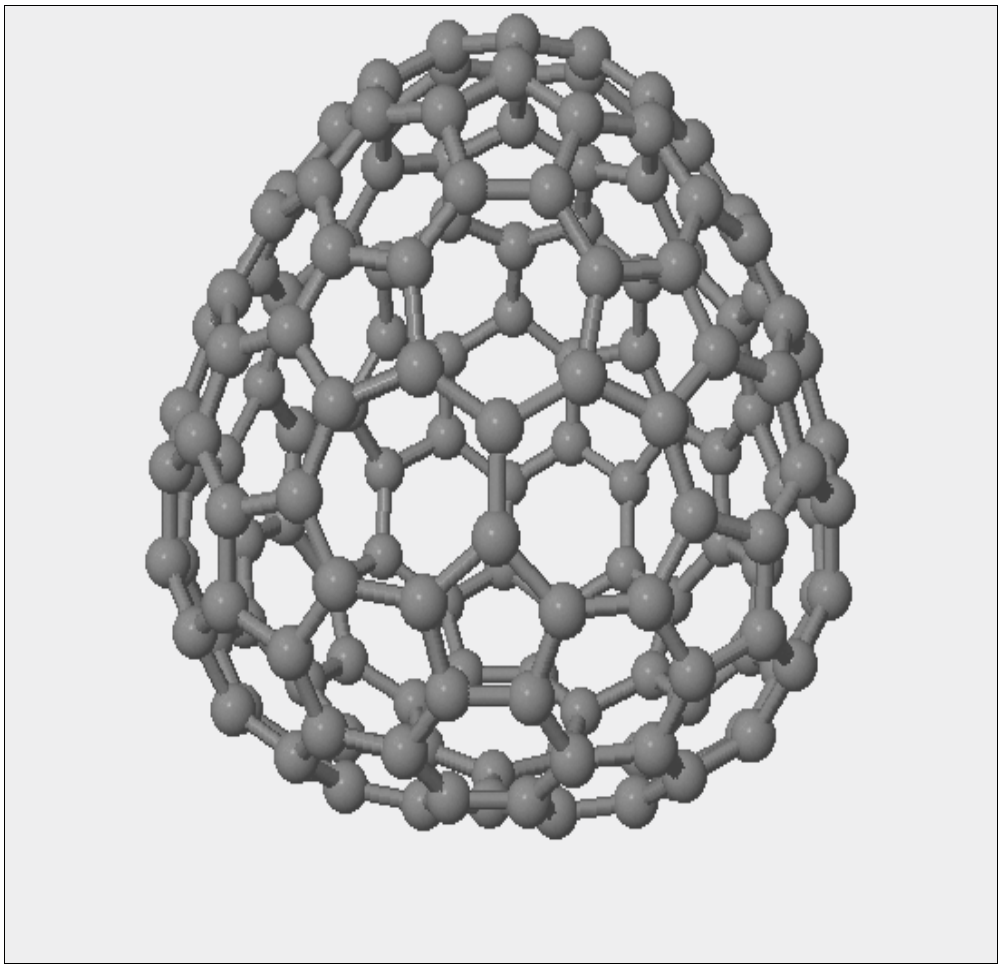

Figure 16. – Face of a nonclassical fullerene with 152 carbons

Each face of this fullerene includes three heptagons, six pentagons, and six hexagons. Between two faces we have one hexagon, and there are six of those hexagons. At each of the four vertex of the fullerene, we find a group of three hexagons. Thus, coming

from the four faces, we take into account 12 heptagons, 24 pentagons, and 24 hexagons. From the boundaries of the faces, we have 6 hexagons, and 12 hexagons from the vertex. Therefore, we have a total number of 12 heptagons, 24 pentagons, and 42 hexagons for this nonclassical fullerene C_{152}.

Discussion

The first fullerene that we presented contains 56 carbons, with 18 hexagons, and 12 pentagons, or a total number of 30 faces.

Our next fullerene it not classical because contains 12 squares, besides 10 hexagons, and 12 pentagons. The number of carbons is 64 with 32 faces.

Now, we consider a fullerene with 76 carbons. In this case, we have 4 hexagons, 24 pentagons, and 12 heptagons, that is, 40 faces.

The fourth fullerene is not classical with 16 hexagons, 24 pentagons, and 6 pentagons. The number of carbons is 88, with 46 faces.

Finally, we consider a fullerene with 152 carbons. In this case, we have 42 hexagons, 24 pentagons, and 12 heptagons, that is, 78 faces.

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Рукапіс паступіў у рэдакцыю