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FULLERENES WITH STRUCTURE OF CUBIC AND OCTAHEDRAL TYPE

Several fullerenes that resemble Cubic or Octahedral structure are presented, between them a molecule with 128 carbons, and another one with 132.

Calculations

Fullerenes with cubic structure look like a box, and we will distinguish a lateral face, with same structure that the opposite face. Also, we will consider the top of the box and its bottom, both of them with the same structure. Finally, we are going to describe the structure of the frontal face, with the same structure that the face located backwards of the box.

The first example that we consider of a classical fullerene contains 72 carbons (figure 1). A lateral face is formed by a central column of two hexagons (with a pentagon at the top, and another one at the bottom) and, at each side a column of three hexagons, giving 8 hexagons, and two pentagons for this face.

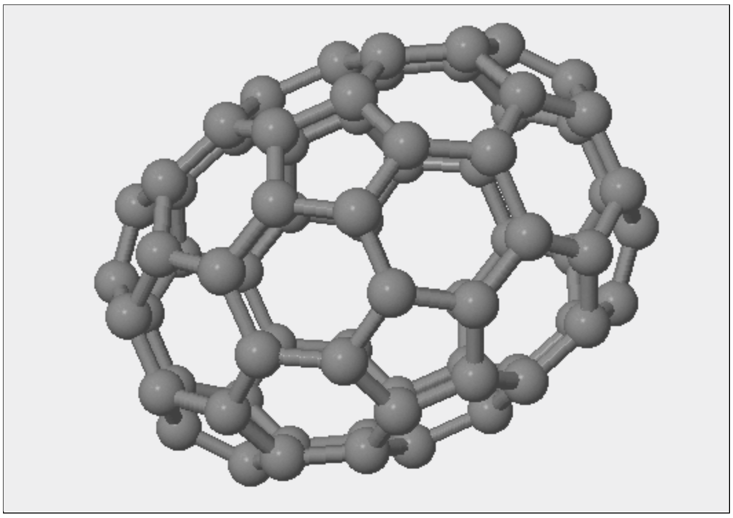

Figure 1. – Lateral face of a fullerene with 72 carbons

The top only provides a row of four hexagons. We observe in figure 2 that this fullerene does not satisfy the isolated pentagon rule.

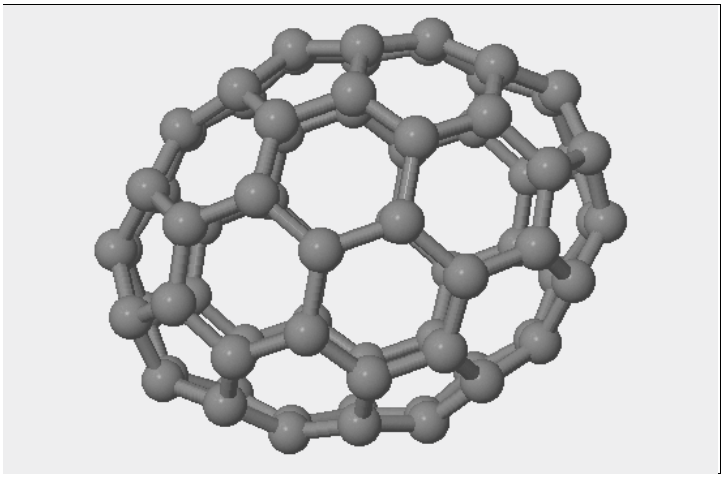

Figure 2. – View from the top of fullerene C_{72}

On the other hand, the frontal face has only one hexagon, and four pentagons (figure 3).

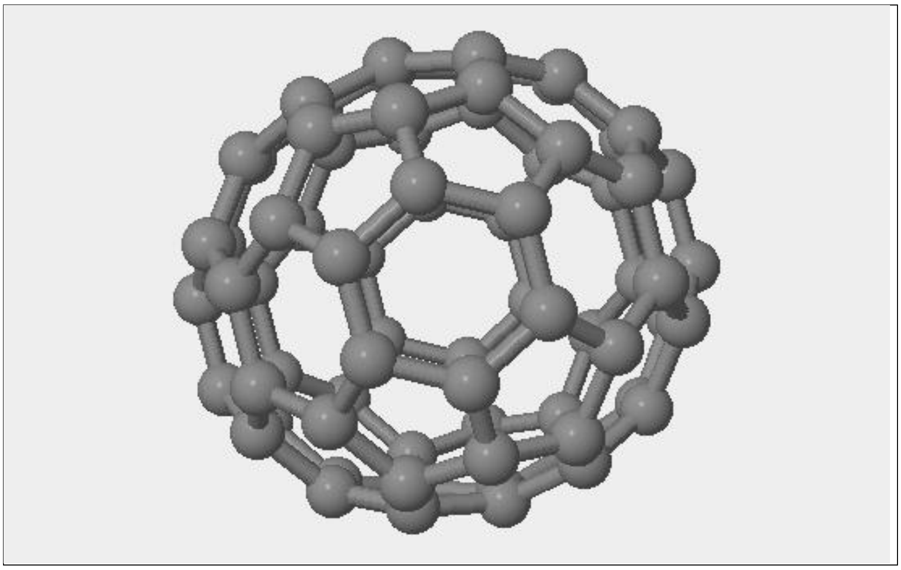

Figure 3. – Frontal face of a classical fullerene with 72 carbons

Therefore, the lateral faces provides 16 hexagons, and 4 pentagons. Then, the top and the bottom provide 8 hexagons, and finally, the frontal, and its opposite face adds two hexagons, and 8 pentagons. Thus, we have 26 hexagons, and 12 pentagons.

Our next molecule contains heptagons. Thus, it is an example of a nonclassical fullerene. We have 128 carbons, 12 pentagons, 30 hexagons, and 12 heptagons, too (figures 4, 5)

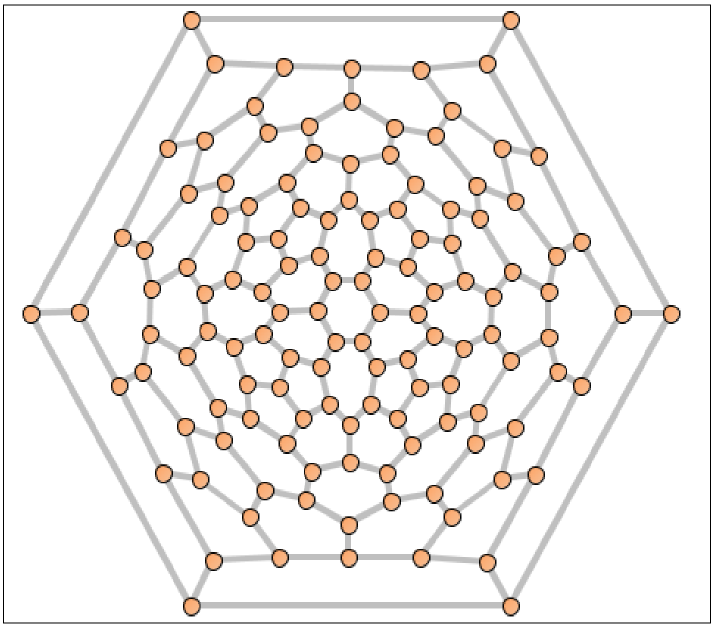

Figure 4. – Schlegel diagram of a nonclassical fullerene with 128 carbons

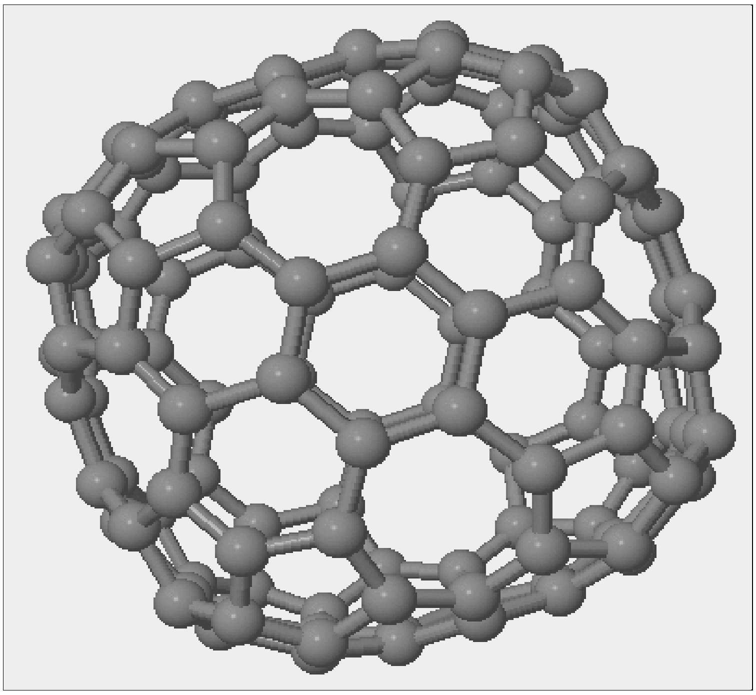

Figure 5. – Lateral face of fullerene C_{128}

The Schlegel diagram of a fullerene with 132 carbons, is shown in figure 6. At the central part, we can observe one hexagon, with 6 neighbours, that are also hexagons. Meanwhile, at the central part of molecule of figure 7, we locate a central hexagon surrounded by 3 heptagons, and 3 pentagons. Actually, figure 6 shows face at the back of the face composed by one hexagon surrounded 6 hexagons displayed on figure 6.

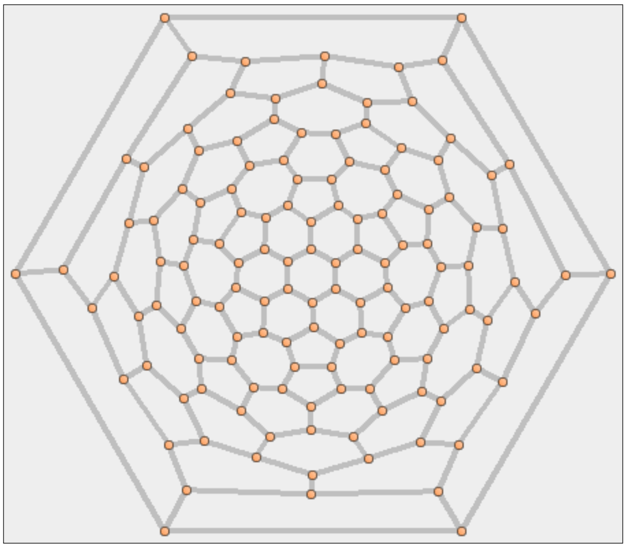

Figure 6. – Schlegel Diagram of a nonclassical fullerene with 132 carbons

We observe too, in figure 6, three couples of pentagons around the central part. Also, we have another close to the top, (12 o'clock) another couple of pentagons at 4 and 5 o'clock; finally, we a couple of pentagons at 7 and 8 o'clock.

Thus, we get 12 pentagons coming from these six couples of pentagons.

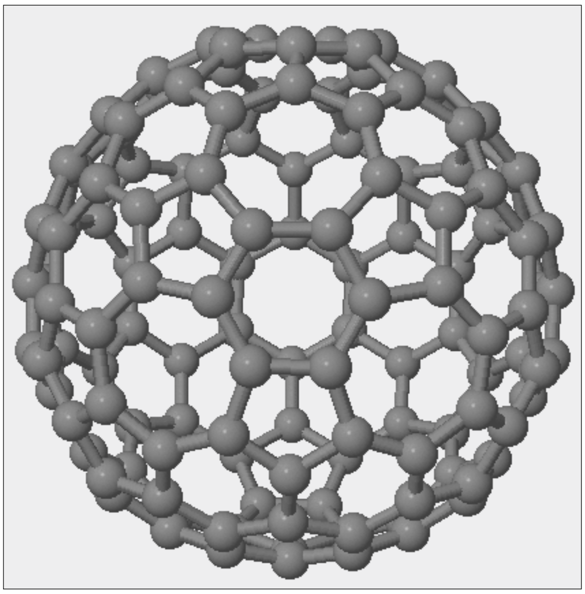

Figure 7. – Nonclassical fullerene with 132 carbons

Since we have two types of faces, the first one with seven hexagons, and there four faces with that structure, we take into account 28 hexagons.

There are also four faces of the other type, each of them adds one hexagon, three heptagons, and 3 pentagons, obtaining four hexagons, 12 heptagons, and 12 pentagons.

Therefore, considering the two types of faces, and the six couples of pentagons, we have a total number of 32 hexagons, 24 pentagons, and 12 heptagons.

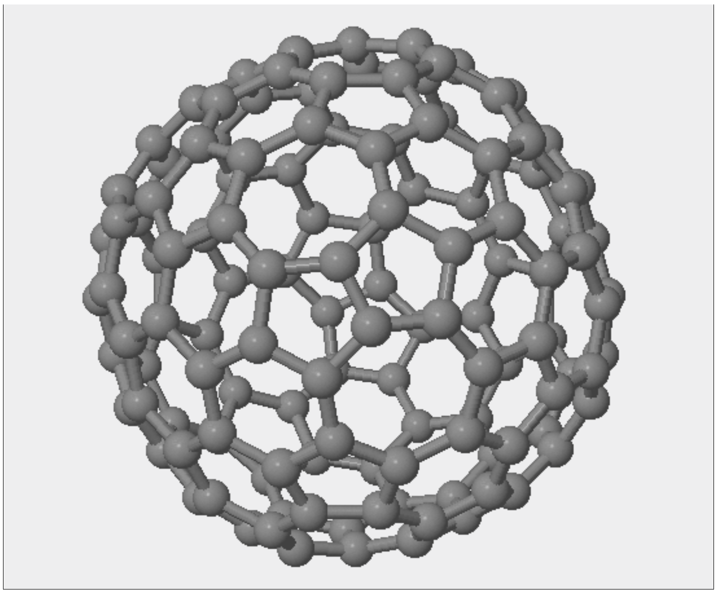

Figure 8. – Another view a nonclassical fullerene with 132 carbons

Our next fullerene has 152 fullerenes, and contains 66 hexagons and 12 pentagons (figures 9–11).

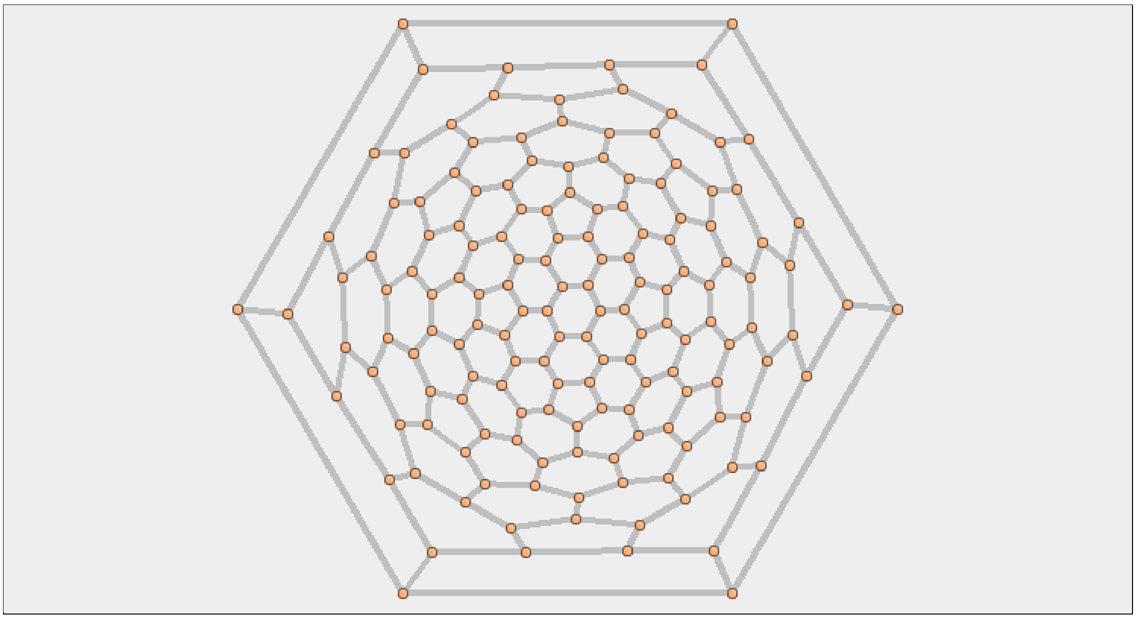

Figure 9. – Schlegel Diagram of a fullerene with 152 carbons

In this construction, a lateral face is formed by six hexagons surrounding one hexagon located at the center. At the upper side of this face we have a pentagon pointing towards the face that form the top of this fullerene. Similarly, we have another pentagon at the lower side of the face, that is pointing towards the face that form the bottom of this fullerene.

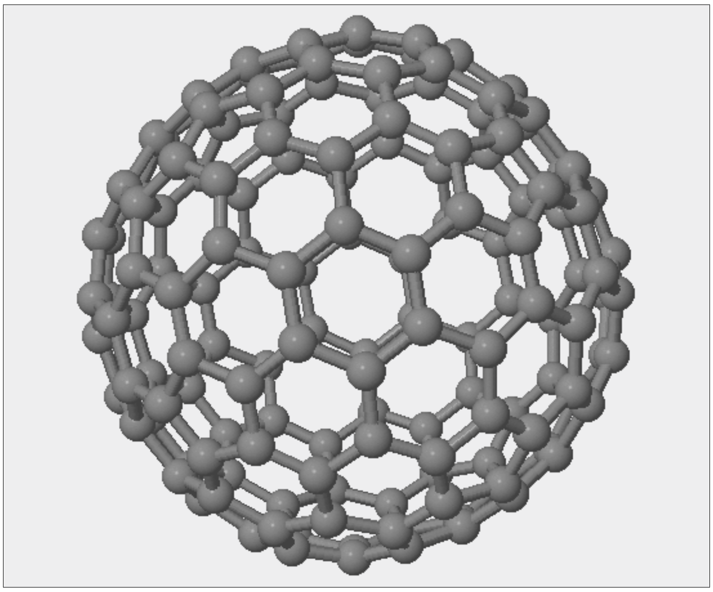

Figure 10. – One of the six faces of a classical fullerene with 152 carbons

The face that we are describing is connected on the left hand side with another face that has a pentagon that is pointing towards the lateral face. In a similar way, the lateral face is connected on the right hand side with another face that has a pentagon that is pointing towards the lateral face. To summarize, our lateral face contains seven hexagons, and four pentagons that are shared with the faces at the top, the bottom, and faces on the left hand side, and the right hand side.

Moreover, between three faces, we have a region formed by three hexagons that is connected with two hexagons of each of the three faces. Also, this region is connected with three pentagons. We can consider this region of three hexagons like a corner of our fullerene.

Counting the number of hexagons of the fullerene, we realize that we have six faces each of them containing seven hexagons. The number of pentagons in opposite sides is four, giving eight pentagons, plus four additional pentagons, for a total number of twelve pentagons, as expected in a classical fullerene.

This fullerene has eight corners, with three hexagons in each of these corners. Therefore, we have six faces with seven hexagons, giving forty two hexagons, plus twenty four hexagons coming from the corners. Thus, we have 66 hexagons, and of course, 12 pentagons for this 152 carbons classical fullerene.

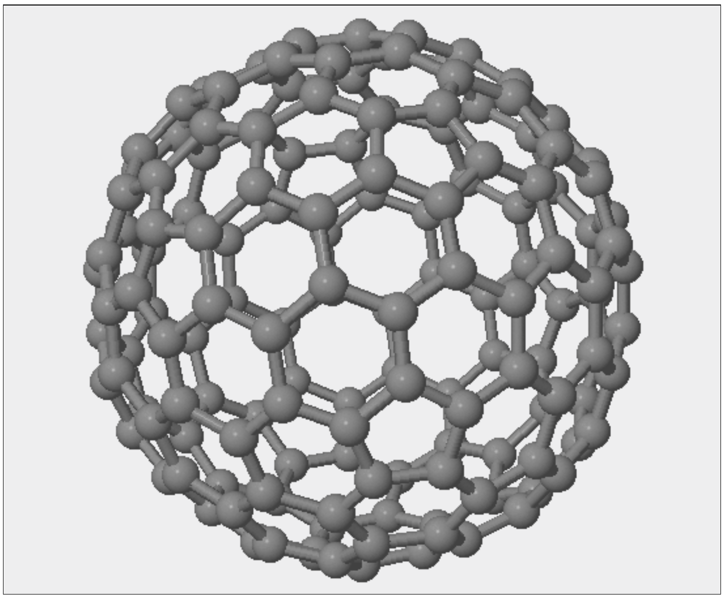

Figure 11. – One of the eight corners of a classical fullerene with 152 carbons

Now, we consider a fullerene with 156 carbons (figure 12). A lateral face is formed by a central column of four hexagons and at each side a column of three hexagons and a couple of outer columns of two hexagons, giving 14 hexagons plus four pentagons at each corner.

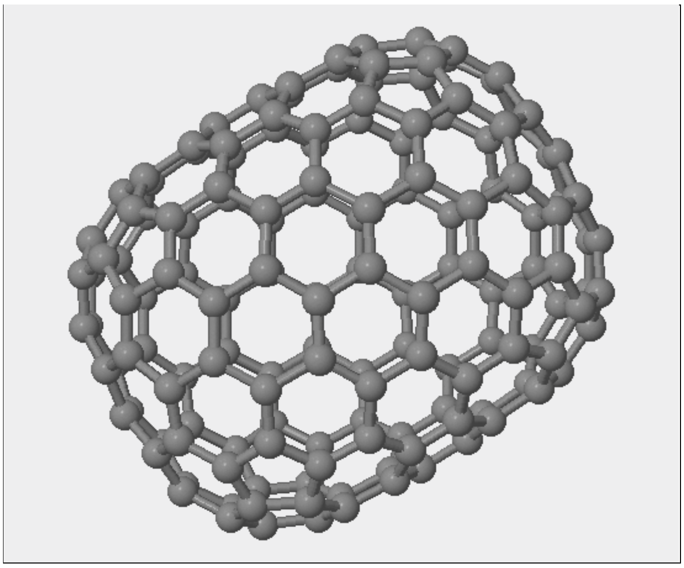

Figure 12. – Lateral face of a classical fullerene with 156 carbons

The top consists of a central column of two hexagons and at each side a column of three hexagons and a couple of outer columns of two hexagons, giving 12 hexagons (figure 13).

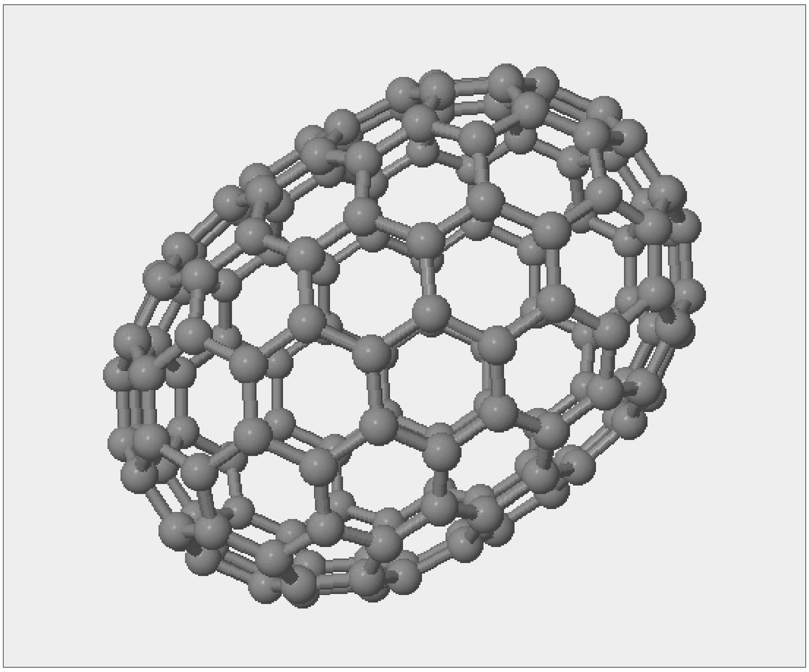

Figure 13. – Upper face of a classical fullerene with 156 carbons

The frontal part of this fullerene is formed by a central column of two hexagons (with a pentagon at the top, and another one at the bottom) and at each side a column of three hexagons, producing 8 hexagons, plus two pentagons (figure 14).

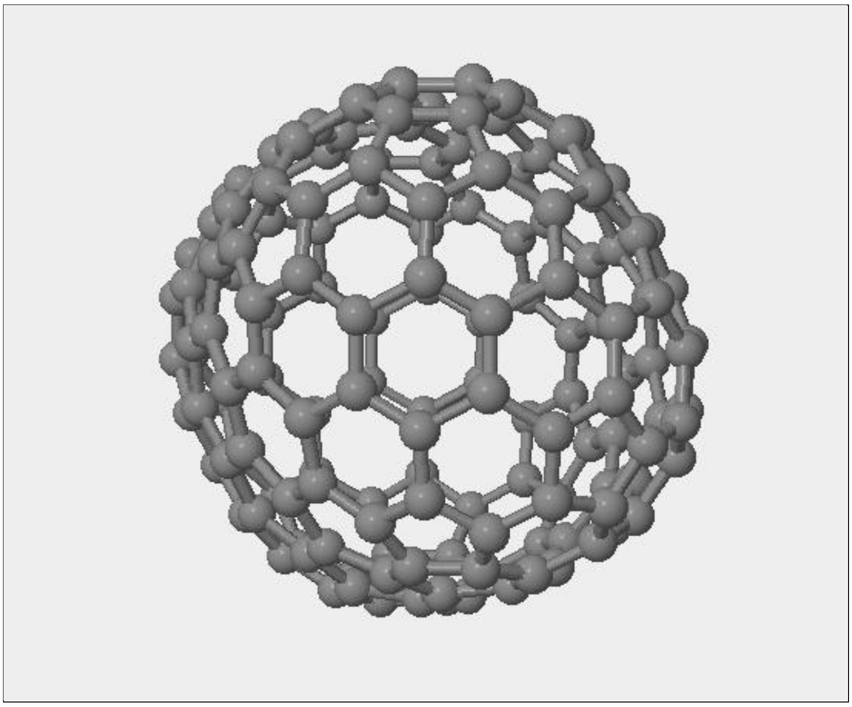

Figure 14. – Frontal face of a classical fullerene with 156 carbons

Since we have two lateral faces, we have to take into account 28 hexagons plus 8 pentagons. Moreover, the top and the bottom contribute with 24 hexagons. Finally, the frontal and the opposite part add 16 hexagons, plus 4 pentagons. Therefore, we have a total number of 68 hexagons, plus 12 pentagons.

Discussion

The first fullerene that we presented contains 72 carbons, with 26 hexagons, and 12 pentagons.

Our next fullerene it not classical because it contains 12 heptagons, besides 30 hexagons, and 12 pentagons. The number of carbons is 128.

Now, we consider a fullerene with 132 carbons. In this case, we have 32 hexagons, 24 pentagons, and 12 heptagons.

The fourth fullerene is classical with 66 hexagons, and 12 pentagons. The number of carbons is 152.

Finally, we consider a fullerene with 156 carbons. In this case, we have 68 hexagons, and 12 heptagons.

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