ON SOME FULLERENES WITH SEVEN HEPTAGONAL RINGS

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Abstract

Four fullerenes with seven heptagonal rings are considered. The first one contains 130 carbons, the second one 134 carbons. Both additional fullerenes has 192 carbons. The fullerene with 130 carbons satisfies the isolated pentagon rule, the fullerene with 134 carbons, does not satisfy the isolated pentagon rule.

Keywords: *nonclassical fullerenes, Schlegel diagram, Isolated pentagon Rule*

1. INTRODUCTION

Study of fullerenes has about three decades [1, p. 162], where the faces of that kind of molecules were found to be hexagons and pentagons. Later, another poligons where considered [2, p. 15634]. Some work has focused in certain geometric properties [3, p. 29], and to consider types of symmetries [4, p. 6], [5, p. 13], that can be analysed by using graph theory [6, p. 58]

2. FULLERENE WITH 130 CARBONS

The first example that is consider is a fullerene with 130 carbons, 19 pentagons, 41 hexagons, and 7 heptagons. A Schlegel diagram of this fullerene is displayed on Figure 1.

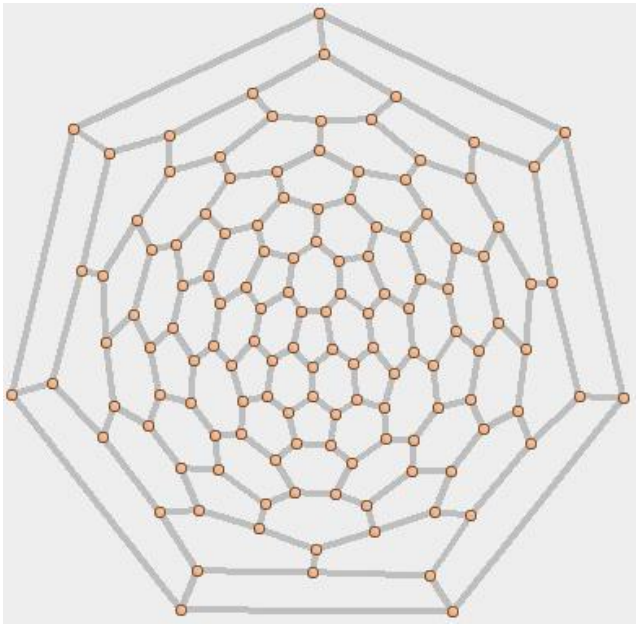


Fig. 1. Schlegel diagram of fullerene C130 with 19 pentagons, 41 hexagons, and 7 heptagons

Structure of this fullerene is based on one hexagon surrounded by another six hexagons and then, three heptagons meet this platform of seven hexagons, as can be seen in Figure 2.

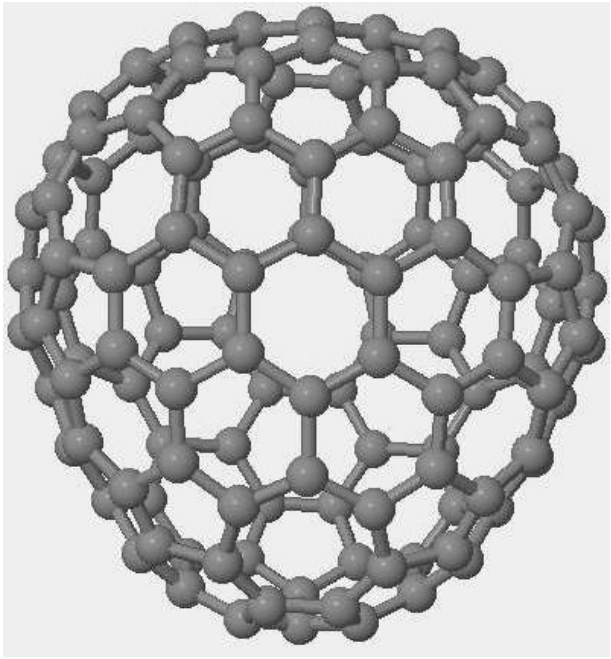


Fig. 2. Bottom region of fullerene C130

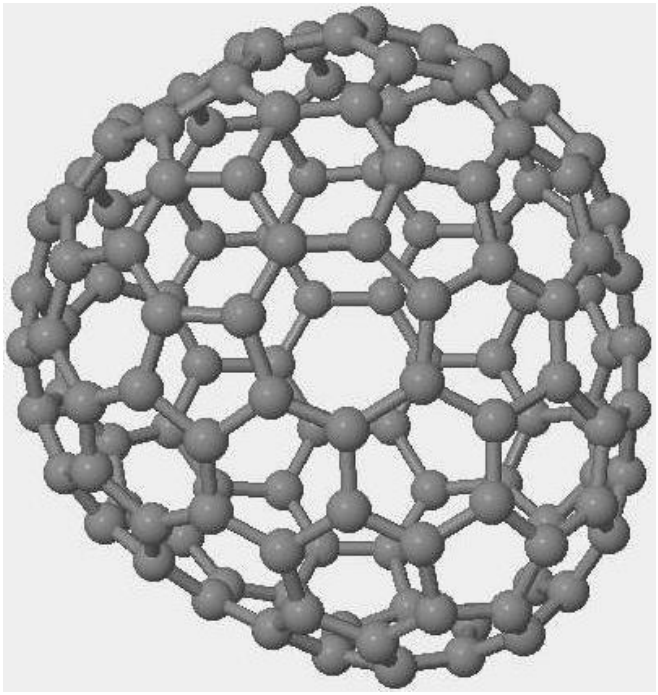


Fig. 3. Upper part of fullerene C130

On the other hand, close to the bottom of Schlegel diagram of Figure 1, there is a heptagon, with a pentagon on each side. That pattern, can be seen on Figure 3, and more clearly on Figure 4. That is, we observe in Figure 4, a heptagon with a couple of hexagons at its base, if we go up, from each side, we meet a pentagon and, at the top, we have three hexagons.

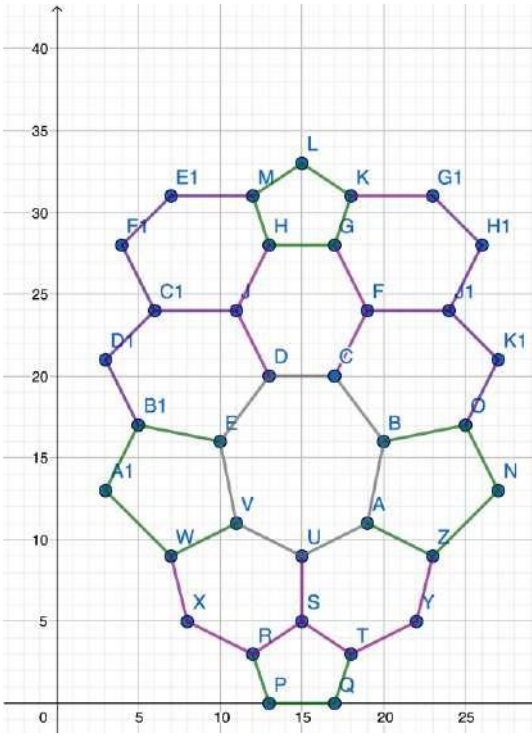


Fig. 4. Basic building block of C130

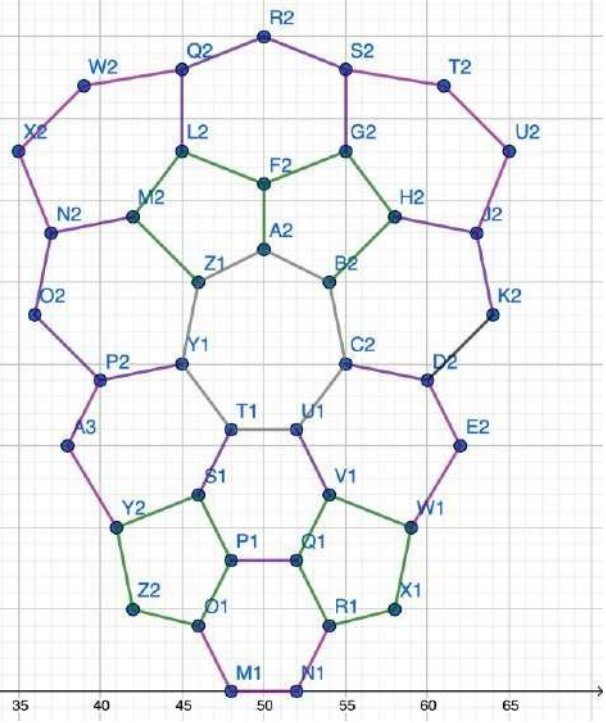


Fig. 5. Basic building block of C134

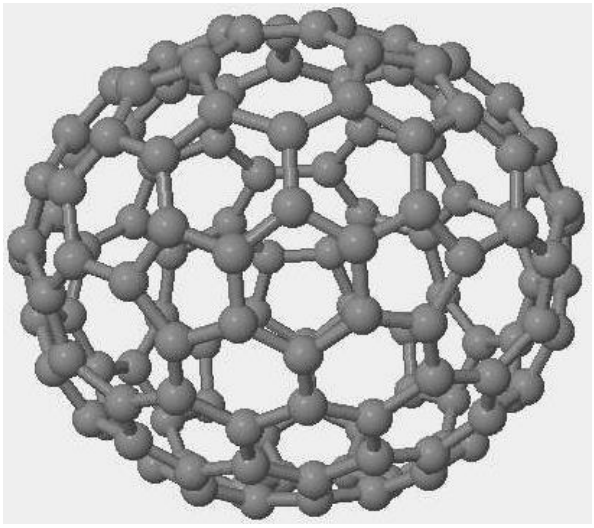


Fig. 6. Back region of fullerene C130

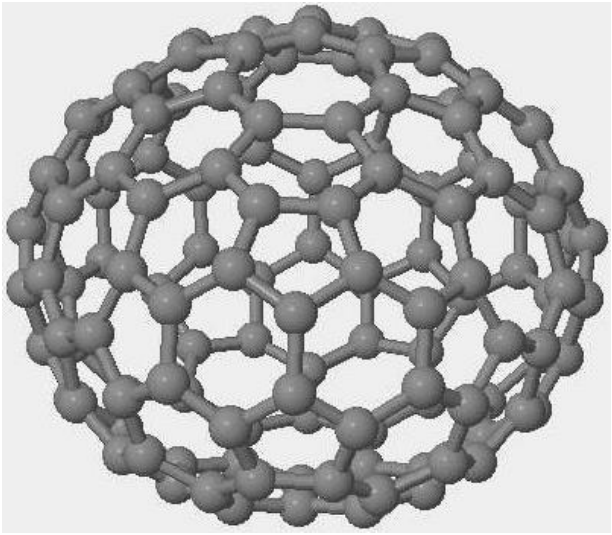


Fig. 7. Frontal region of fullerene C130

Let us look at Figure 4. At the bottom we have pentagon with vertex P, Q, T, S, and R. That same pentagon appears at the top of Figure 6 and meets a heptagon on the upper region of that Figure 6. On the other hand, at the top of Figure 4, we have another pentagon, with vertex K, L, M, H, and G. The same pentagon is located at the center of Figure 7, and is surrounded by six hexagons. Therefore, putting together Figures 2, 3, 6, and 7, oriented by Figure 4, we get an idea of the structure of this fullerene composed by 130 carbons with 19 pentagons, 41 hexagons, and 7 heptagons.

3. FULLERENE WITH 134 CARBONS

Next, structure of polygons that appear in Figure 4 will be modified in the following way. Hexagon with vertex D, C, F, G, H, and J will be substituted by a couple of pentagons. One of them with vertex A2, B2, H2, G2, and F2. The other pentagon with vertex A2, F2, L2, M2, and Z1. Both pentagons are shown on Figure 5. This modification, transforms pentagon with vertex K, L, M, H, and G, that appears on Figure 4 into the hexagon with vertex F2, G2, S2, R2, Q2, and L2 that is located at the top of Figure 5. At this step, the heptagon that originally appears in Figure 4, has become an octagon. In order to recover the heptagon of Figure 4, pentagon with vertex P, Q, T, S, and R, will substituted by hexagon with vertex M1, N1, R1, Q1, P1, and O1. Simultaneously, the linear segment from V to U, and the segment from U to A of Figure 4 are going to be substituted by edge that goes from T1 to U1 of Figure 5. As a consequence, pentagon with vertex A1, W, V, E, and B1, of Figure 4 is transform into hexagon with vertex A3, Y2, S1, T1, Y1, and P2 of Figure 5, and pentagon with vertex A, Z, N, O, and B, of Figure 4 is transform into hexagon with vertex U1, V1, W1, E2, D2, and C2 of Figure 5. Another consequence is that appears hexagon with vertex U1, T1, S1, P1, Q1, and V1 of Figure 5.

Also, hexagon with vertex U, V, W, X, R, and S, of Figure 4 is reduced to pentagon with vertex O1, P1, S1, Y2, and Z2 of Figure 5. Similarly, hexagon with vertex S, T, Y, Z, A, and U, of Figure 4 is reduced to pentagon with vertex Q1, R1, X1, W1, and V1, of Figure 5. This complete the

transformation of Figure 4 into Figure 5, and we observe that the nodes on the boundary of region shown in Figure 4 are P, Q, T, Y, Z, N, O, K1, …, W, X, and R, the number of this nodes is 23. On the other hand, is we count the nodes on the boundary of region shown in Figure 5, we also obtain 23 nodes.

Therefore, the number of nodes on both boundaries, coincide. Next, the chain of carbons at the bottom of Figure 4 is composed by nodes X, R, P, Q, T, and Y. Meanwhile, there is a corresponding chain of carbons at the bottom of Figure 5, that is composed by nodes Z2, O1, M1, N1, R1, and X1. Thus, we can paste to the bottom of structures of both Figures 4 and 5, the structure shown on Figure 6.

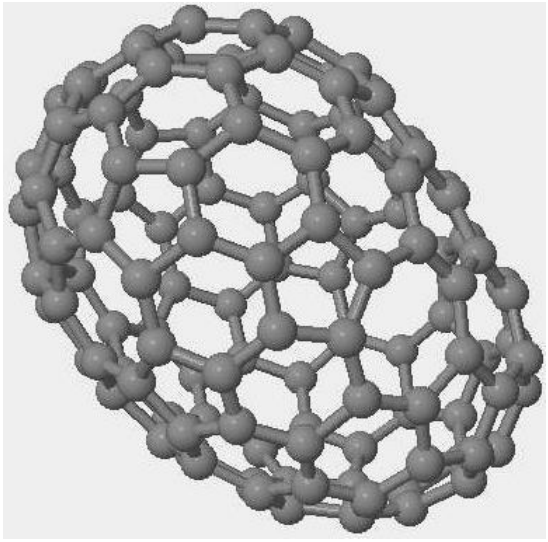


Fig. 8. Lateral region of fullerene C134

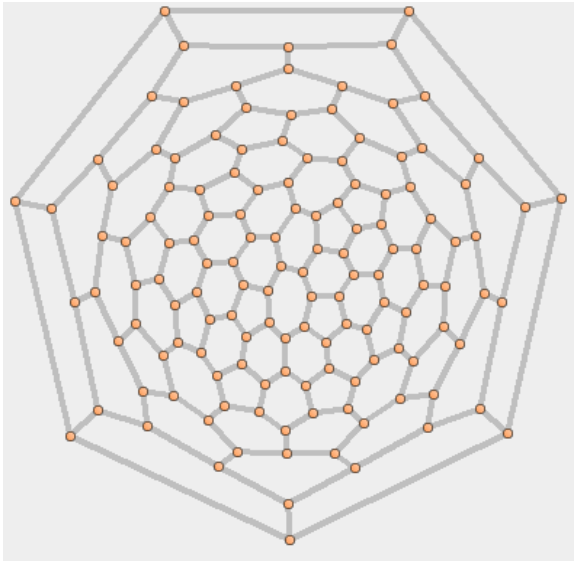


Fig. 9. Schlegel diagram of fullerene C134 with 19 pentagons, 43 hexagons, and 7 heptagons

Similarly, the chain of carbons at the top of Figure 4 is composed by nodes F1, E1, M, L, K, G1, and H1. Meanwhile, there is a corresponding chain of carbons at the top of Figure 5, that is composed by nodes X2, W2, Q2, R2, S2, T2 and U2. Thus, we can paste to the top of structures of both Figures 4 and 5, the structure shown on Figure 7. Therefore, we obtain a fullerene with 134 carbons, that also has 7 heptagons. On Figure 8, it is shown a lateral view that is common to original fullerene C134, and also, to new fullerene C130. Schlegel diagram of C130 is displayed on Figure 9.

At center of Figure 9, there is a heptagon that is connected with another heptagon through a hexagon. This last heptagon meets a couple of pentagons that are located next to each other.

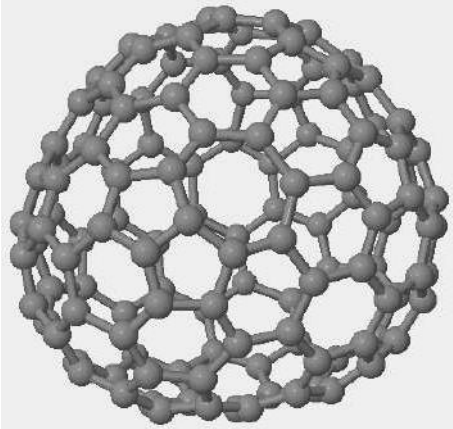


Fig. 10. Fullerene C134

This couple of pentagons can also be observed at center of Figure 10.

4. A COUPLE OF FULLERENES WITH 192 CARBONS

The third example of that is consider is a fullerene with 192 carbons, that contains 19 pentagons, 72 hexagons, and 7 heptagons. A Schlegel diagram of this fullerene is displayed on Figure 11.

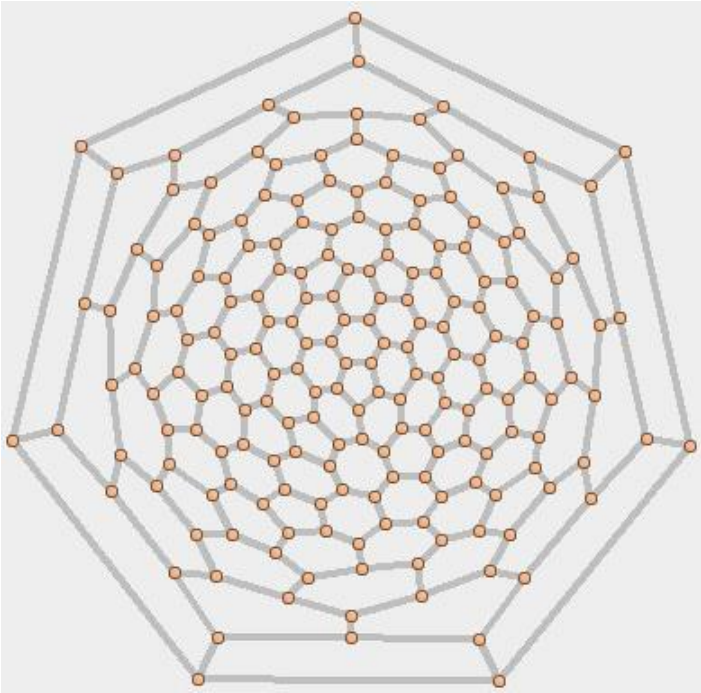


Fig. 11. Schlegel diagram of fullerene C192 with 19 pentagons, 72 hexagons, and 7 heptagons A corresponding three-dimensional representation is shown on Figure 12

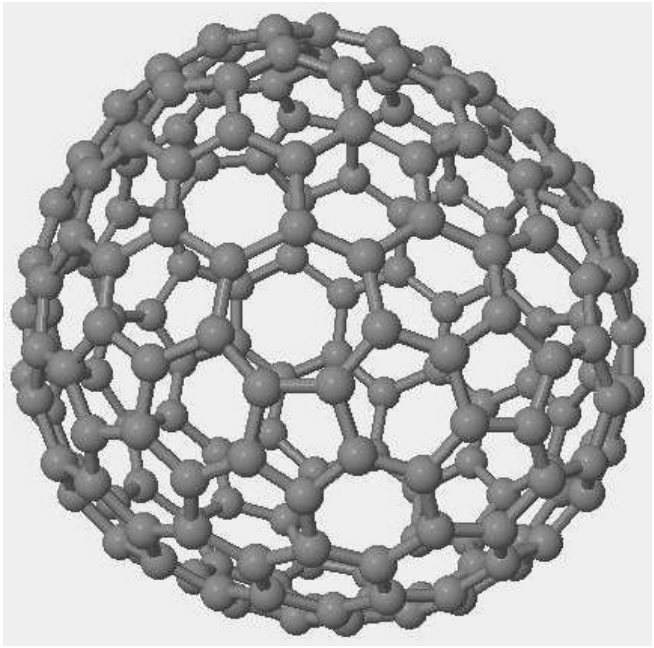


Fig. 12. Fullerene C192 with central heptagon that only meets one pentagon

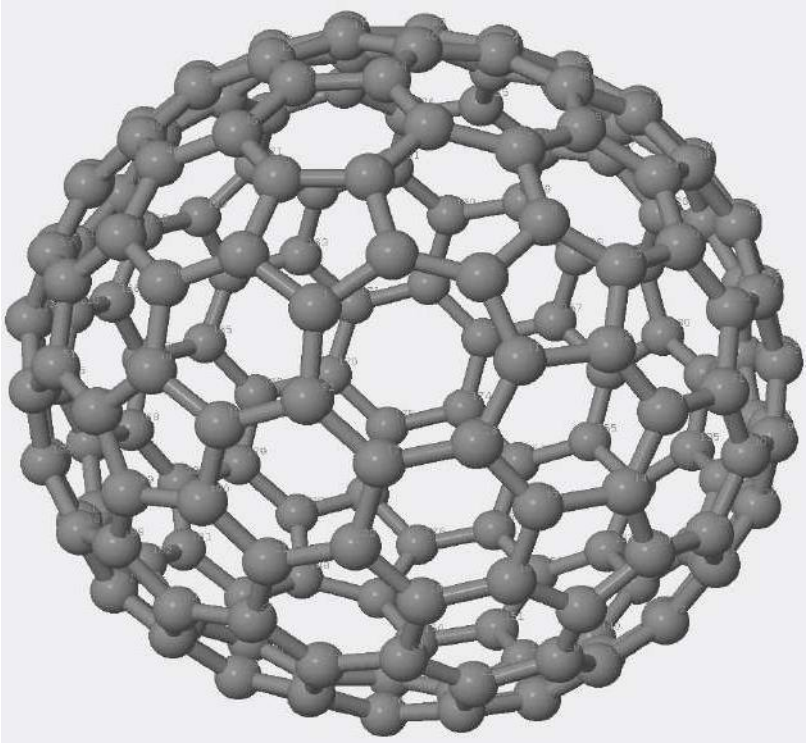


Fig. 13. Fullerene C192 where every heptagon meets at least 2 pentagons

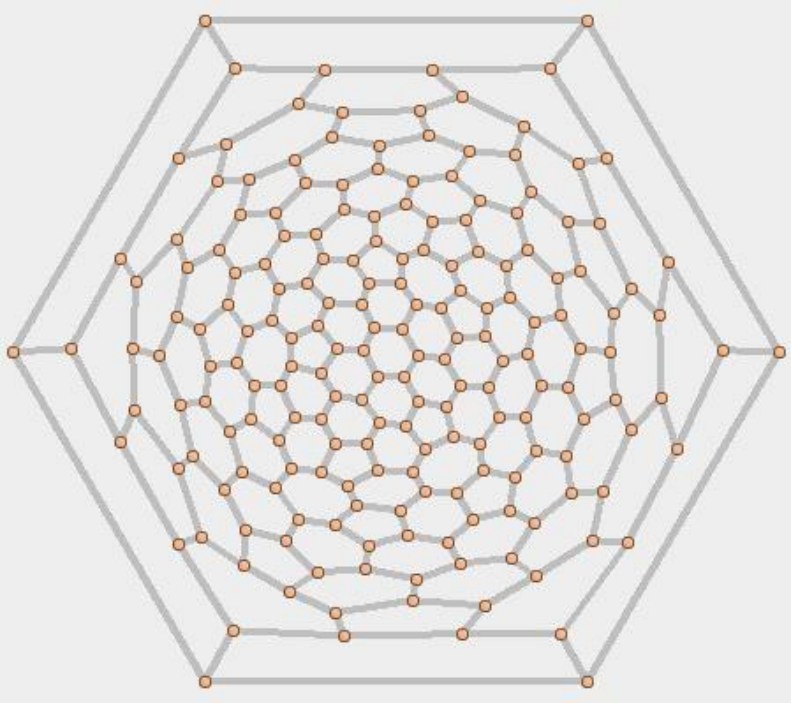


Fig. 14. Schlegel diagram of fullerene C192 with 72 pentagons, 7 heptagons, and 19 pentagons

5. RESULTS

Four fullerenes with seven heptagonal rings are presented. The first one contains 130 carbons, the second one 134 carbons. Both additional fullerenes has 192 carbons. The fullerene with 130 carbons satisfies the isolated pentagon rule, the fullerene with 134 carbons, does not satisfy the isolated pentagon rule.

6. DISCUSSION

Future work will be focused in trying to construct more fullerenes with seven heptagonal rings if all of them contains 19 pentagons. Also, one question is to find fullerenes of this type with the minimal number of carbons.

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