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STRUCTURE AND ENERGY OF THE Δn=6 SERIES FULLERENES

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I. INTRODUCTION

Earlier it was shown that fullerenes can grow by reacting with each other, similar to bubbles in a soap solution [1]. In this case fullerenes C_{24}, C_{32}, C_{40}, and C_{48} can be formed; the structure periodicity being Δn=8, where n is the number of carbon atoms. The periodicity has one and the same main characteristic feature; the fullerene structure changes from threefold symmetry to sixfold through four and fivefold ones. We suppose that this feature can be taken as a basis for rigorous fullerene classification in addition to the geometric classification developed for mini-fullerenes [2].

Now we want to increase the number of fullerenes fitted our classification by adding the fullerenes of the structure periodicity Δn=6 designed in Ref. 3. In this contribution we present the structure and energy of such fullerenes. Knowing their structure allows one to activate the fullerenes, including unknown previously, for farther investigations and use of their properties.

II. FUSION REACTIONS OF CUPOLA HALF FULLERENES

In Ref. [1] we have developed an algorithm that has proved itself in predicting the growth of perfect fullerenes conserving an initial symmetry, so called the fusion reaction algorithm. Consider reactions leading to mini-fullerenes C_{14}. In Fig. 1 the atomic configurations corresponding to reaction $C_7 + C_7 \rightarrow (C_7C_7) \rightarrow C_{14}$ and $C_4 + C_{10} \rightarrow (C_4C_{10}) \rightarrow C_{14}$ are shown. At first two molecules C_7, or C_4 and C_{10}, are moving towards each other (Figs. 1, a and d). Then the boundary atoms (dark-red) interact with each other producing a compound (Figs. 1, b and e). During this process new covalent bonds (heavy red lines) are generated, distorted polyhedrons are formed; they relaxing into perfect polyhedrons (Figs. 1, c and f). In the first case, the atomic configuration consists of six squares and three hexagons so it can be termed a tetra6-hexa3-polyhedron. It should be emphasized that the hexagons have a conformation known for cyclic molecules as a boat [4]. In the second case, the atomic configuration consists of three squares and six pentagons so it can be termed a tetra3-penta6 polyhedron. It is a basic truncated bipyramid. This structure was designed in Ref. 3 on the basis of graph theory.

Reactions leading to mini-fullerenes C18. Analogously consider the atomic configurations corresponding to reactions $C_9 + C_9 \rightarrow (C_9C_9) \rightarrow C_{18}$ and $C_6 + C_{12} \rightarrow (C_6C_{12}) \rightarrow C_{18}$. As before, we have two cases of joining (Fig. 2 a, b. c and Fig, 2, d. e, f). The first case results in the atomic configuration corresponding to a perfect polyhedron that consists of two equilateral triangles, six pentagons, and three hexagons, so it could be named a tri2-penta6-hexa3 polyhedron; the hexagons having a boat conformation. In the second case an isomer of fullerene is obtained; it is an all-vertices truncated triangular bipyramid.

Reactions leading to midi-fullerenes C_{24} are $C_{12} + C_{12} \rightarrow (C_{12}C_{12}) \rightarrow C_{24}$ and $C_8 + C_{16} \rightarrow (C_8C_{16}) \rightarrow C_{24}$ (Fig. 3). The final atomic configuration in the fist case is a perfect polyhedron that consists of two squares, eight pentagons, and four hexagons, i.e. a tetra2-penta8-hexa4 polyhedron; the hexagons having a boat conformation. In the second case an isomer of fullerene C_{24}, a truncated octahedron (cuboctahedron), is obtained.It is worth noting that the cavities formed in f.c.c. metals by irradiation are also coboctahedra bounded by {100} and {111} planes [5].

Reactions leading to midi-fullerenes C_{30}. can be written as $C_{15} + C_{15} \rightarrow (C_{15}C_{15}) \rightarrow C_{30}$ and $C_{10} + C_{20} \rightarrow (C_{10}C_{20}) \rightarrow C_{30}$. Their visualization is presented in Fig. 4. In the fist case the final atomic configuration is a perfect polyhedron of twelve pentagons and five hexagons, so it could be named a penta12-hexa5 polyhedron; the hexagons having also a boat conformation. In the second case it is a truncated pentagonal bipyramid.

Reactions leading to midi-fullerenes C_{36}, are $C_{18} + C_{18} \rightarrow (C_{18}C_{18}) \rightarrow C_{36}$ and $C_{12} + C_{24} \rightarrow (C_{12}C_{24}) \rightarrow C_{36}$ (Fig. 5). In the fist case the final atomic configuration is a perfect polyhedron of twelve pentagons and fourteen hexagons, so it could be named a penta12-hexa14 polyhedron; the hexagons having also a boat conformation. In the second case it is a truncated hexagonal bipyramid.

SINGLE AND DOUBLE BONDS, ENERGY

We assume that the symmetry of double bonds location about the major axis of cupolas and other fullerenes coincides with that of fullerene C60. Using this postulate, we have all the necessary input data for the optimization of the fullerene structures. The optimized structures of these fullerenes obtained through the use of Avogadro package [6] are shown in Fig. 6. We have also calculated formation energies of the fullerenes (Fig. 6).

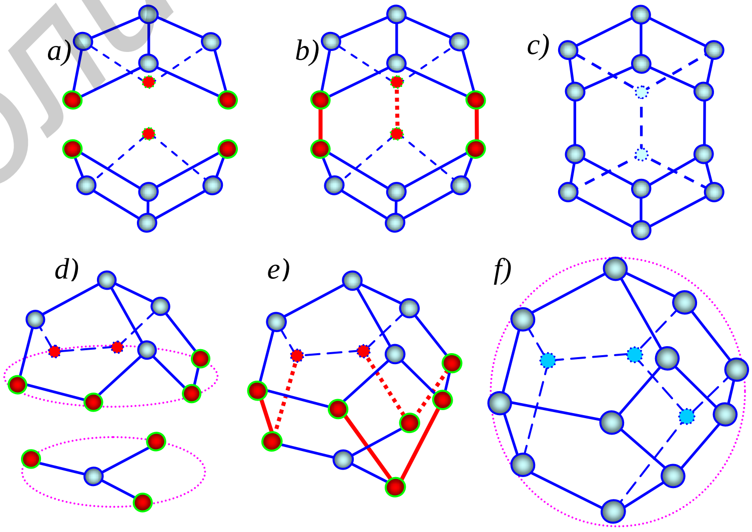

Figure 1 – C_{14} as joining two cupolas C_7 (a, b, c) and cluster C_4 with cupola C_{10} (d, e, f); Dark-red and light-blue balls are reacting and neutral atoms, respectively; solid and dashed red lines are new covalent bonds

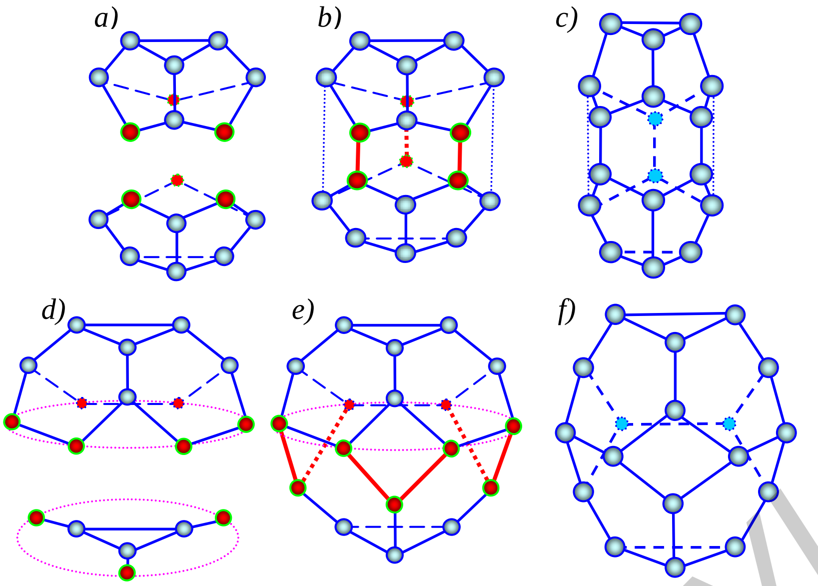

Figure 2 – C_{18} as joining two cupolas C_9 (a, b, c) and plane cluster C_6 with cupola C_{12} (d, e, f); notations are the same as before

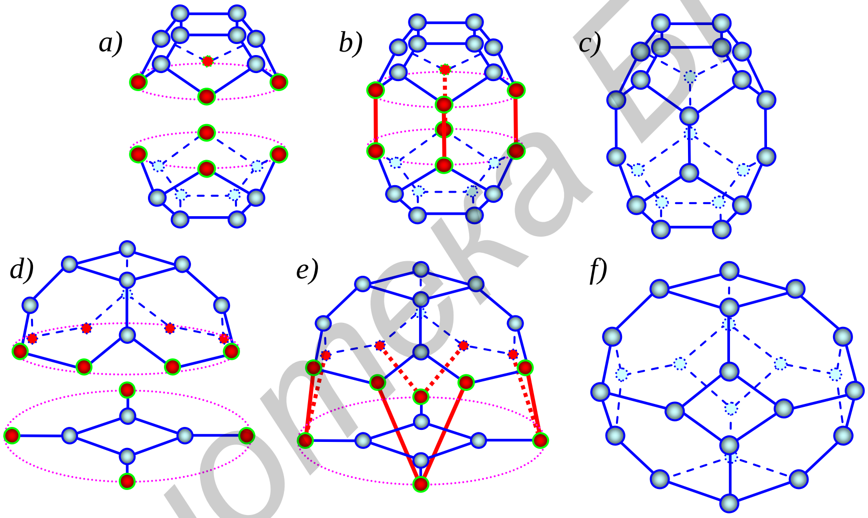

Figure 3 –C_{24} as joining two cupolas C_{12} (a, b, c) and plane cluster C_8 with cupola C_{16} (d, e, f); notations are the same as before

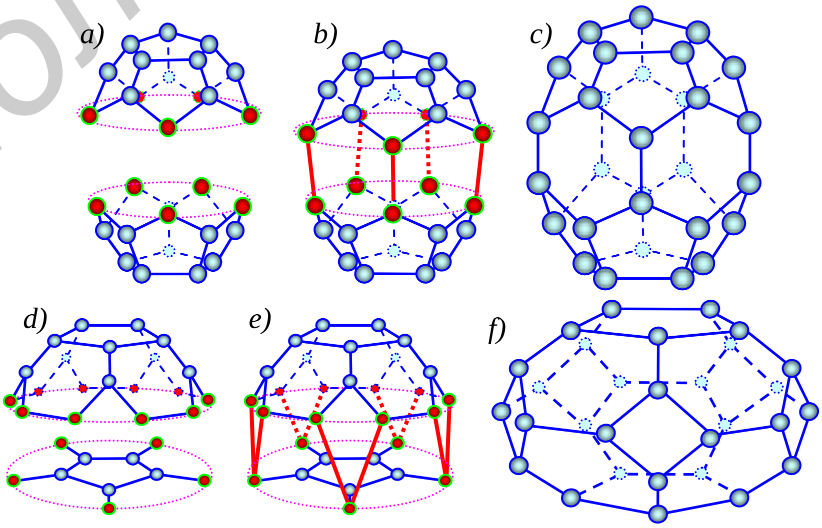

Figure 4 – C_{30} as joining two cupolas C_{15} (a, b, c) and plane cluster C_{10} with cupola C_{20} (d, e, f); notations are the same as before

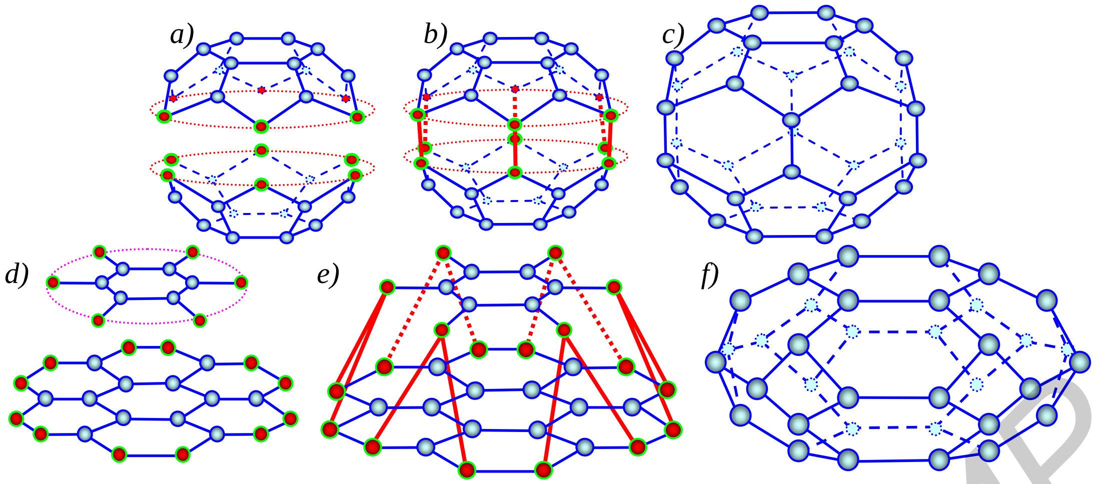

Figure 5 – C_{36} as joining two cupolas C_{18} (a, b, c) and two graphene fragments C_{12} and C_{24} (d, e, f); notations are the same as before

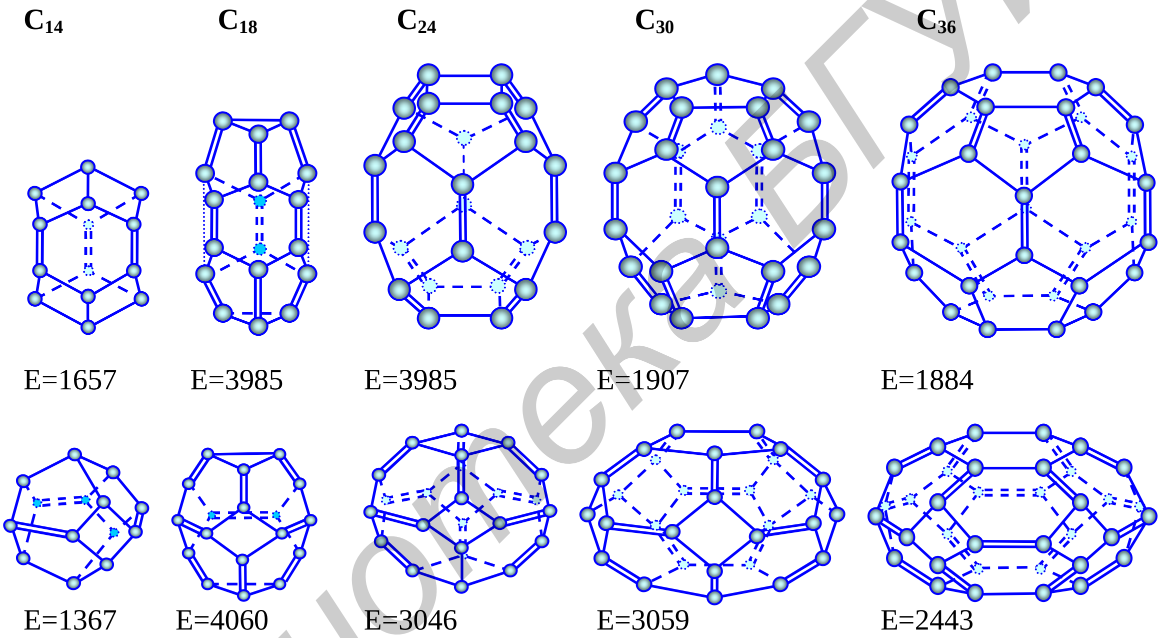

Figure 6 – Structure and energy (kJ/mol) of the Δn=6 series fullerenes with single and double bonds

The energy change for fullerenes can be explained in the following manner. According to two of five basic empirical arguments [7], “geodesic structural factors should favor the more symmetric isomers, which can evenly disperse the strain from bond-angle deformation. This suggests that only 5/6–ring networks are likely to occur readily”. Really, this is reflected in the energy of fullerenes C_{14} (below), C_{30} and C_{36} (above), but is invalid for C_{14} (above). We see that the rather low energy obtained unexpectedly contradicts to these arguments and needs more careful investigation. We suppose that in this case self-organization of unshared electron pairs (physical factor) [8] prevails over decreasing the ellipticity (mathematical point of view).

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STRUCTURE AND ENERGY OF THE Δn=14 SERIES FULLERENES

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I. INTRODUCTION

Fullerenes can be imagined to grow by reacting with each other, similar to bubbles in a soap solution. In Ref. [1] we considered this possibility using geometrical modeling and have found the Δn=8 periodicity for the family fullerenes originating from the reactions $C_{10}+C_{10}$. Later on we found that the fullerenes can create the Δn=6, Δn=10, and Δn=12 periodicities. All these periodicities have one and the same main characteristic feature; the fullerene structure changes from threefold symmetry to sixfold through four and fivefold ones. Taking this feature as a basis for fullerene classification, we have suggested the periodic system for such fullerenes. It consists of horizontal series and vertical columns (groups). The horizontal series form the Δn periodicities considered, the vertical columns include the fullerenes of the same symmetry, the mass difference Δm for each column being equal to a double degree of symmetry. We suppose that the fullerenes of one and the same group have similar properties.

In addition to the series Δn=8, Δn=10 and Δn=12, the fullerene stricture of which was designed elsewhere, we added to the system other series. The fullerene structure for the series Δn=14 and Δn=16 was also obtained through the use of geometric modeling, but the results were not published. In this contribution we present the structure and energy of the Δn=14 series fullerenes. Knowing these characteristics allows one to activate the fullerene for farther investigations.

II. FUSION REACTIONS OF CUPOLA HALF FULLERENES

In Ref. [1] we have developed an algorithm that has proved itself in predicting the growth of perfect fullerenes conserving an initial symmetry, so called the fusion reaction algorithm. Reaction between two cupolas C_{16} and C_{22}. In Fig. 1 the atomic configurations corresponding to reaction $C_{16}+C_{22}\rightarrow(C_{16}C_{22})\rightarrow C_{38}$ are shown. At first two molecules are moving towards each other (Fig. 1, a). Then the atoms, marked in dark-red, interact with each other producing a compound (Fig. 1, b). During this process new covalent bonds (heavy red lines) are being formed. As a result, a distorted polyhedron is formed which relaxes into a perfect polyhedron (Fig. 1, c). Its atomic configuration consists of nine hexagons and twelve pentagons, so it can be was named a penta12hexa9-polyhedron.

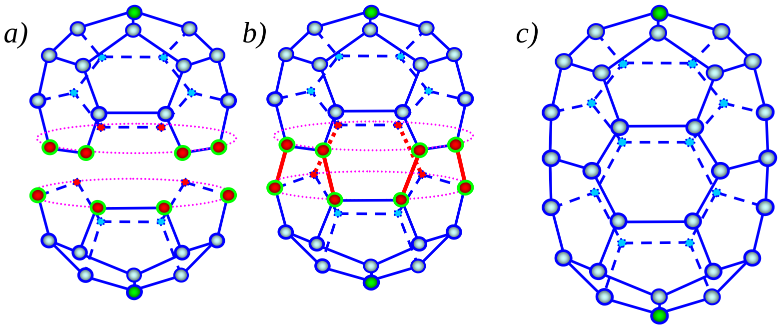

Figure 1 – Joining of two half-fullerenes C_{16} and C_{22};
a) Separate carbon cupolas; b) Intermediate compound; c) Penta12hexa9-polyhedron C_{38} after relaxation.
Dark-red and light-blue balls are reacting and neutral atoms, respectively; thin light-blue solid and dashed lines are covalent bonds; heavy dark-red solid and dashed lines are new covalent bonds.