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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.

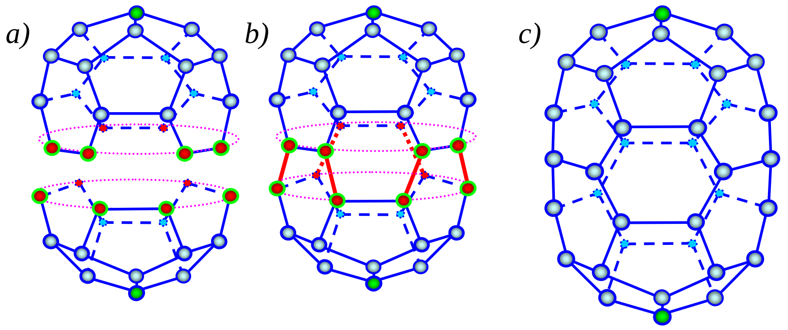


Figure 1 – Joining of two half-fullerenes C_{16} and C_{22};
a) Separate carbon cupolas; b) Intermediate compound; c) Penta12hexa9-polyhedron C_{38} after relaxation.
Dark-red and light-blue balls are reacting and neutral atoms, respectively; thin light-blue solid and dashed lines are covalent bonds;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

Reaction between two cupolas C_{18} and C_{24}. Similar to the previous reasoning, one can consider the atomic configurations corresponding to reaction $C_{18} + C_{24} \rightarrow (C_{18}C_{24}) \rightarrow C_{42}$. As before, at first two molecules are moving towards each other (Fig. 2, a). Then the boundary atoms interact with each other producing a distorted polyhedron (Fig. 2, b), which relaxes into a perfect polyhedron (Fig. 2, c). Its atomic configuration consists of two triangles, six pentagons and fifteen hexagons and so it can be was named a tri2penta6hexa15-polyhedron.

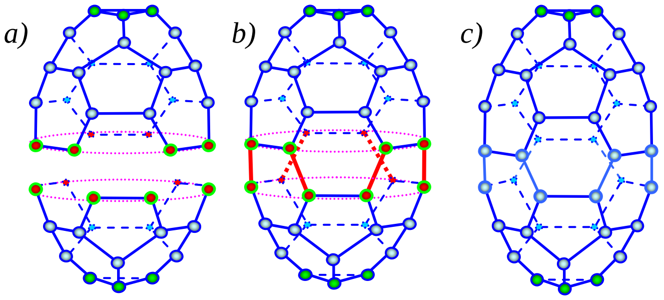


Figure 2 – Joining of two half-fullerenes C_{18} and C_{24}; notations are the same as before

Reaction between two cupolas C_{24} and C_{32}. The procedure for visualization of reaction $C_{24} + C_{32} \rightarrow (C_{24}C_{32}) \rightarrow C_{56}$ is the same as before. The atomic configuration of the perfect polyhedron (Fig. 3, c) consists of two squares, eight isolated pentagons and twenty-two hexagons, so it could be named a tetra2-penta8-hexa22-polyhedron.

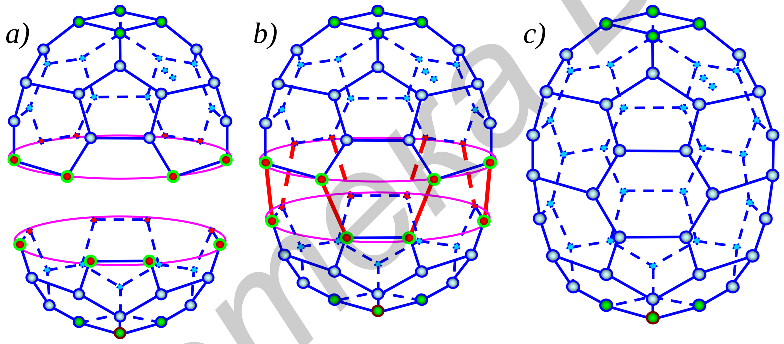


Figure 3 – Joining of two half-fullerenes C_{24} and C_{32}; notations are the same as before

Reaction between two cupolas C_{30} and C_{40} is written as $C_{30} + C_{40} \rightarrow (C_{30}C_{40}) \rightarrow C_{70}$.The atomic structure corresponding to a perfect polyhedron (Fig. 4, c) consists of twelve isolated pentagons and twenty-five hexagons, so it could be named a penta12-hexa25 polyhedron. Its graph and the graphs of reacting cupolas are also shown in Fig. 4.

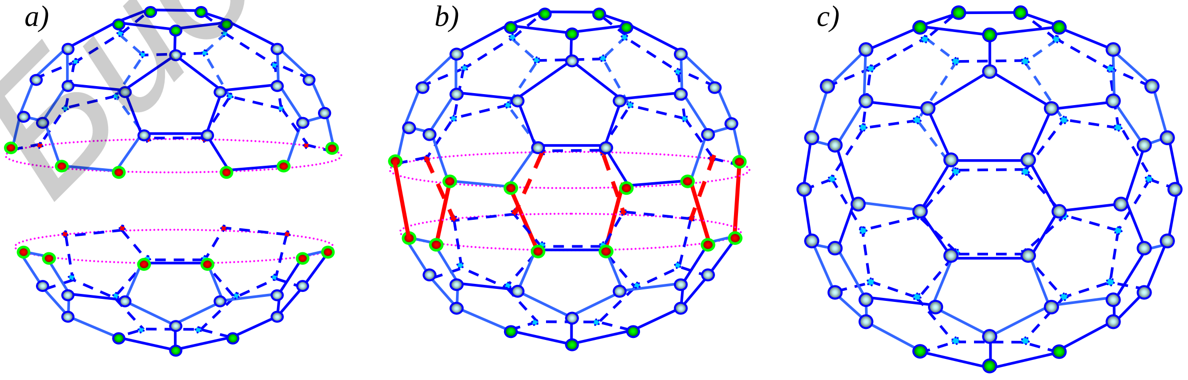


Figure 4 – Joining of two half-fullerenes C_{30} and C_{40}; notations are the same as before

Reaction between two cupolas C_{36} and C_{48}. The procedure for visualization of reaction $C_{36} + C_{48} \rightarrow (C_{36}C_{48}) \rightarrow C_{84}$ is the same as before. The atomic structure corresponding to a perfect polyhedron (Fig. 5, c) consists of twelve isolated pentagons and thirty-two hexagons, so it could be named a penta12-hexa32 polyhedron,

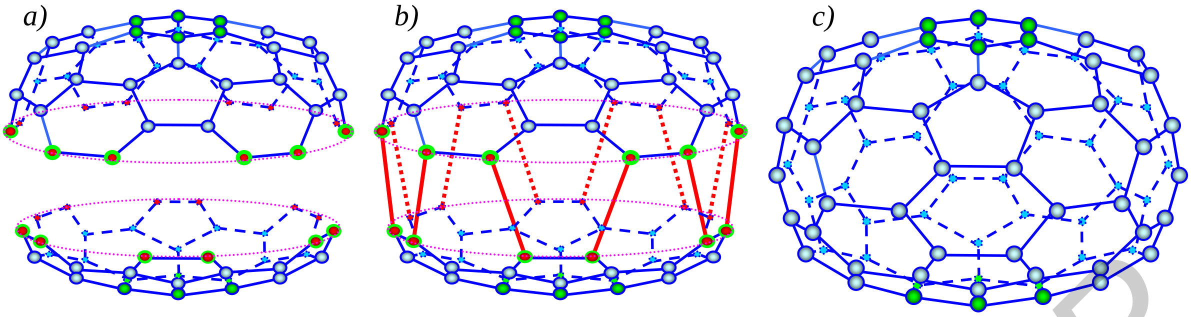


Figure 5 – Joining of two half-fullerenes C36 and C48; notations are the same as before

III. SINGLE AND DOUBLE BONDS

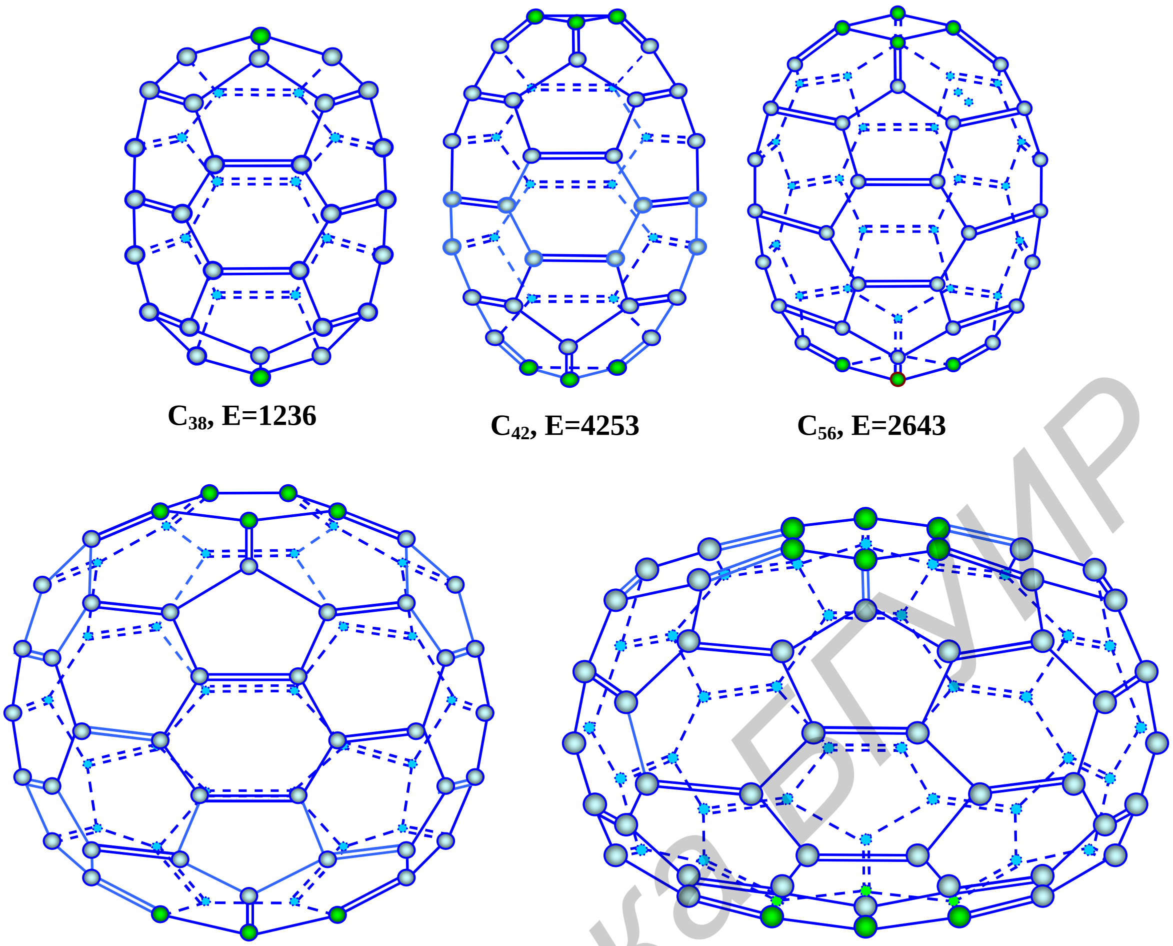
We assume that the symmetry of double bonds location about the major axis of cupolas and other fullerenes coincides with that of fullerene C_{60}. Using this postulate, we have all the necessary input data for the optimization of the fullerene and cupola structures designed by means of geometric modeling and for subsequent calculation of their properties. As it was described above, the cupolas having one and the symmetry can react with each other producing fullerenes C_{36}, C_{48}, C_{60}, and C_{72} with single and double covalent bonds and, in the case of fullerene C_{32}, with partially delocalized bonds too. The optimized structures of the fullerenes obtained through the use of Avogadro package [2] are shown in Fig. 6. The energy change for the fullerenes can be explained in a similar manner as in Ref. 3.

IV. DISCUSSION

Today there are a lot of papers on fullerene properties. Using different computational methods (there are also a lot of programs), the authors calculate the properties of the most popular fullerenes which structure is known. As a result, the numbers obtained contradict to each other and only increase disordered information. The absence of appreciable progress in understanding fullerene nature is determined by the domination of numerical calculations on the known structures. However, any numerical calculations are unable to predict new structures, so the 'numerical progress' results mainly in increasing numerical entropy. It should be emphasized that numerical calculations are not a theory, but a kind of numerical experiment [4].

Consequently, it is necessary not to do calculations for calculations, but at first to develop a system (mathematical model) as a basis for the calculations. The first step of creating any mathematical model is the formulation of the laws that connect the main objects of the model [5]. In our case the main objects are perfect basic fullerenes; we have also the preliminary law in the form of the periodic system [6] and the fusion algorithm for obtaining perfect basic fullerenes, but we do not know the structure of all the main objects. Besides, not all perfect fullerenes, the structure of which being known, are incorporated in the suggested periodic system.

Therefore, the next step in our investigation is obtaining the structure and energy of missing fullerenes with the purpose to incorporate the missing known and unknown fullerenes in the periodic system. Only afterwards, having a comprehensive picture, it seems reasonable to try to explain why some fullerenes are more stable than others.



C_{38}, E=1236 C_{42}, E=4253 C_{56}, E=2643

C_{70}, E=2069 C_{84}, E=2255

Figure 6 – Structure of the Δn=14 series fullerenes with single and double bonds. Energy in kJ/mol

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ON OPTIMIZATION OF HYDROGENERATOR THRUST BEARING CHARACTERISTICS

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I. INTRODUCTION

In conditions of the world hydropower dynamic development and construction of a large number of hydro power plants in developing economics: Brazil, China, India, etc. it is important to ensure reliable trouble-free operation of the key structural elements of the plant.