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# Nucleation and growth of fullerenes and nanotubes having five-fold symmetry

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**Abstract**. We have studied possible ways of generating and growing the fullerenes having five-fold symmetry. Beginning with cyclopentane $C_5H_{10}$ and clusters $C_5C_5$, we obtained elementary fullerenes $C_{10}$ and mini-fullerenes $C_{20}$, and then we produced the fullerenes from $C_{20}$ to $C_{70}$, perfect (basic) and imperfect, as well as nanotubes. The basic fullerenes $C_{20}$, $C_{30}$, $C_{40}$, $C_{50}$, $C_{60}$, and $C_{70}$ have the ordinary five-fold symmetry, the intermediate ones having no such symmetry. Their imperfection is connected with extra 'interstitial' carbon dimers, the dimers playing the role of defects. One can define the imperfect fullerenes with defects as the fullerenes having topological five-fold symmetry. We have calculated the energies of both groups of fullerenes and discussed their dependence on a fullerene size and shape.
**Keywords**: carbon, embedding, energy, fullerene, fusion reaction, graph representation, growth, nanotube, periodic system, single and double bonds, topological symmetry

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## 1. Introduction

In our early investigations we have tried, as most investigators, to study some popular fullerenes, e.g. $C_{20}$, $C_{24}$, $C_{36}$, $C_{60}$, and $C_{70}$, to calculate their energy and to do some conclusions about their stability and other properties. However, with the passage of time, we came to the conclusion that such a style of investigation leads to a dead end. The reason is that these fullerenes have different symmetry and belong to different columns of the periodic table of fullerenes suggested in [1,2]. Moreover, in those cases the main rule of an experiment is violated: the data must be obtained and compared, all other things or factors being equal or the same. It should be emphasized that numerical calculations are not a theory, but a kind of numerical experiment [3]. So such calculations in many cases only increase information entropy [4].

Consequently, there is little sense in doing calculations for the sake of calculations, but at first, one needs to develop a plan and a mathematical model of calculations. It should be pointed out that the mathematical model is meant not a computational method employed, but the interplay between physical processes expressed through mathematics. The first stage 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 law in the form of the periodic table, but we do not know the structure of all the main objects.

Besides, not all the perfect fullerenes, the structure of which is known, are incorporated into the established periodic system. Therefore, it seems reasonable to carry out such studying that allows obtaining the structure of missing fullerenes, with the purpose to incorporate the missing unknown fullerenes in the periodic table, and only afterward to do conclusions, bearing in mind that all the factors being equal or the same.

The periodic table of fullerenes [1,2] consists of horizontal series and vertical columns (groups); they include basic perfect fullerenes from $C_{14}$ to $C_{96}$. The horizontal series form the $\Delta n$ periodicities, where the fullerene structure changes from three-fold symmetry to six-fold through four and five ones. The vertical columns include the fullerenes of one and the same symmetry, the mass difference $\Delta m$ for each column being equal to a double degree of symmetry. We declare that the periodic system must be taken as a base for rigorous fullerene classification. The system leaves room for incorporating into it other fullerene families.

In this contribution, we have studied the nucleation and growth of the fullerenes referring to the column of five-fold symmetry. Similar investigations were done earlier for fullerenes of three-fold [6] and four-fold symmetry [7].

## 2. Embryos, clusters, folding, fusion, and formation of fullerenes and nanotubes

We assume that the embryo of fullerenes of five-fold symmetry is cyclopentane $C_5H_{10}$ with $D_{5h}$ symmetry [8]. Suppose that we have removed ten hydrogen atoms and added five carbon atoms instead. In doing so we obtain carbon cluster $C_5C_5$ with several types of carbon atoms. They are shown, together with cyclopentane $C_5H_{10}$, in Fig. 1. We have calculated the optimized structures and energy of these compounds as well as of the succeeding ones through the use of Avogadro package [9]. The carbon atoms of cyclopentane remain in the initial electronic state; they are considered, as is customary, to be $sp^2$ hybridized atoms. The newly added ones are reactive carbon atoms; they are connected with the initial carbon atoms by single or double bonds, being ionized to a different degree. The further cluster evolution is folding and forming a penta-angular prism (Fig. 2).

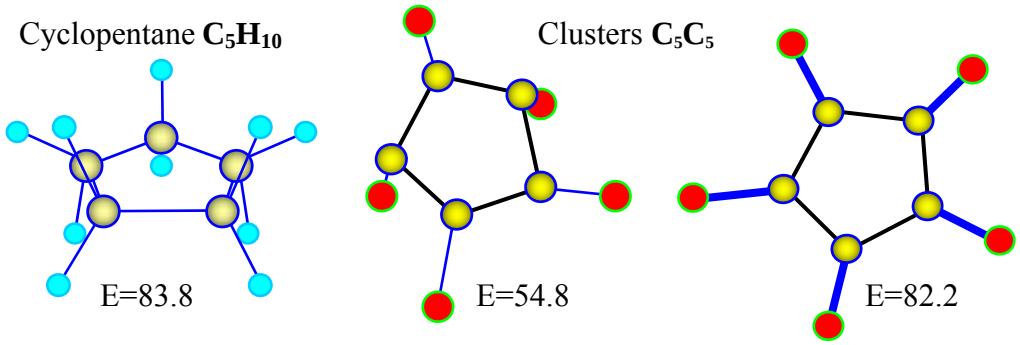



**Fig. 1** Cyclopentane and two carbon clusters of five-fold symmetry; energy in kJ/mol

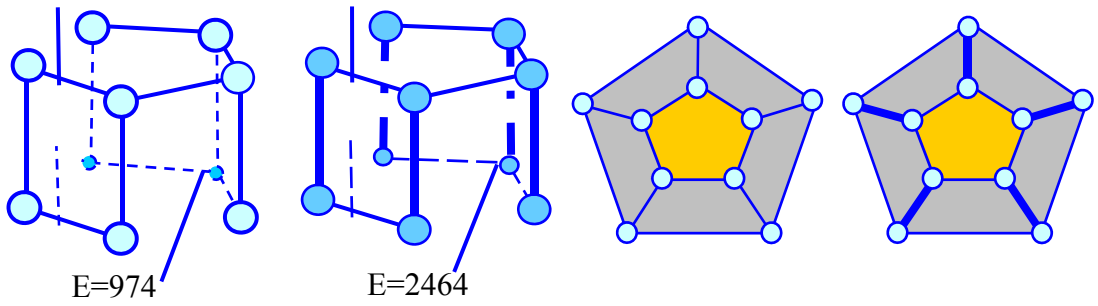



**Fig. 2.** Folding the clusters into pentagonal prisms: structure and graphs; energy in kJ/mol

Consider cluster folding more closely. The process produces the elementary fullerene of five-fold symmetry which is a pentagonal prism. Two extreme electronic configurations are presented in Fig. 2. In addition to the structures, the graphs of prisms are shown. Here and below we use area-colored graphs because they gain a better understanding of the structures obtained. In our case all the side faces of prisms are tetragons and they are grey painted in graphs; the upper faces are pentagons and they are painted in goldish; the bottom faces are indicated by the external boundaries.

The elementary fullerenes can grow, conserving their symmetry, by the mechanism known as the "fusion of fullerenes having compatible symmetry" [10]. The final structure produced by the fusion of two prisms is shown in Fig. 3. The shape of the fullerene is a dodecahedron. It is one of five regular polyhedrons that Plato (427-347 BC) referred to as ether. It enters into the family of barrel-shaped fullerenes, so-called "mini-fullerenes".

In its turn this fullerene can continue growing and conserve the symmetry, only through the use of the above-mentioned mechanism, i.e. joining another prism (Fig. 4). The reaction is possible since the reacting structures have five-fold symmetry and therefore they are compatible with each other. The subsequent fusion of the fullerenes is presented in Fig. 5. The hexagons in the graphs are painted in yellow.

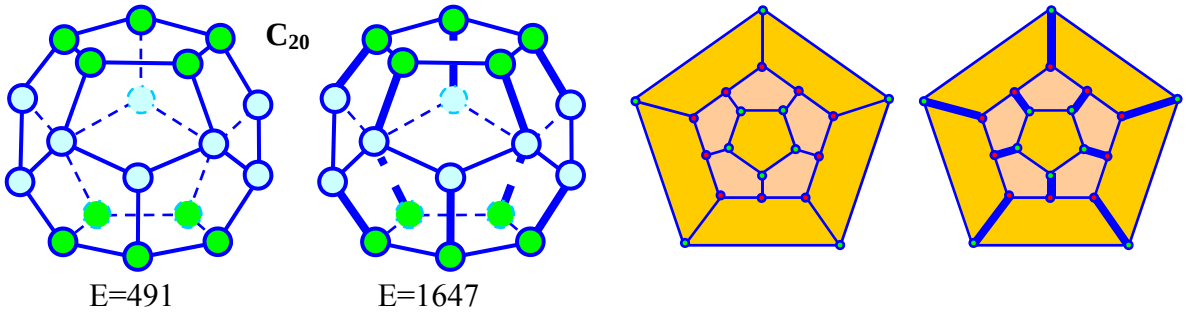



**Fig. 3**. Dodecahedron $C_{20}$ as a result of prisms fusion; its graphs and energy in kJ/mol

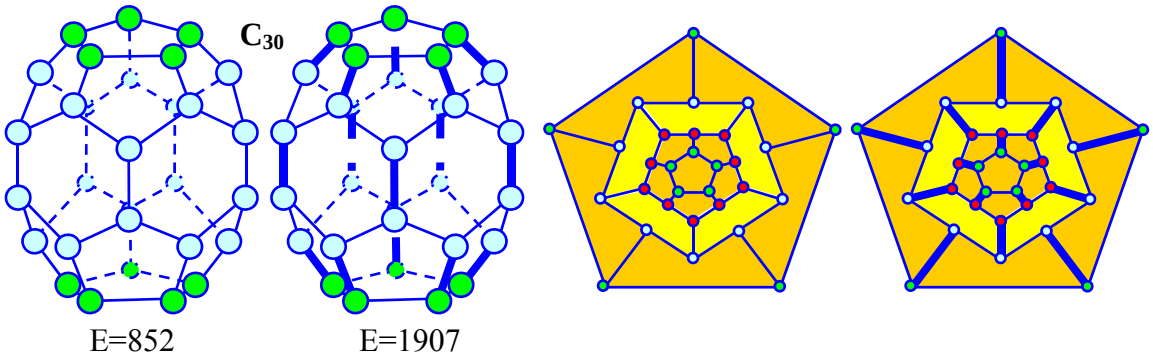



**Fig. 4**. Joining dodecahedron to a prism; structure, graphs, and energy in kJ/mol

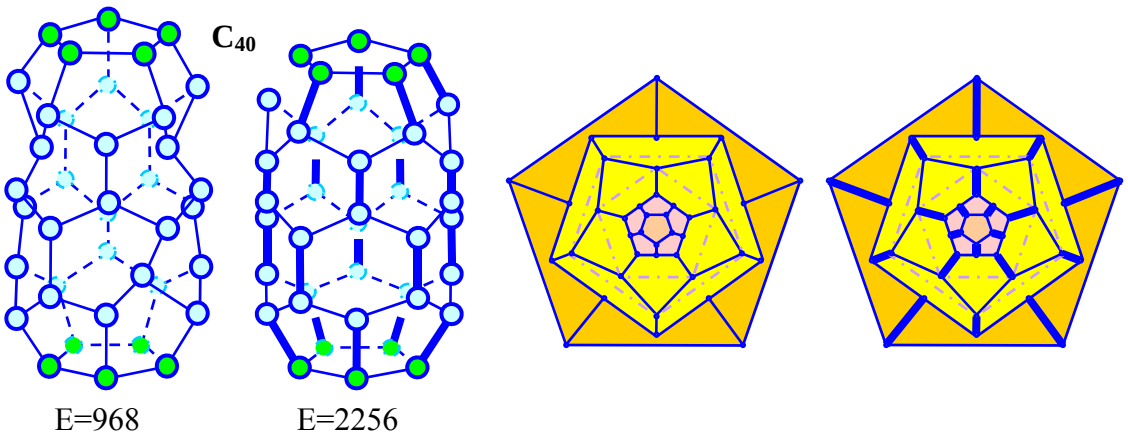
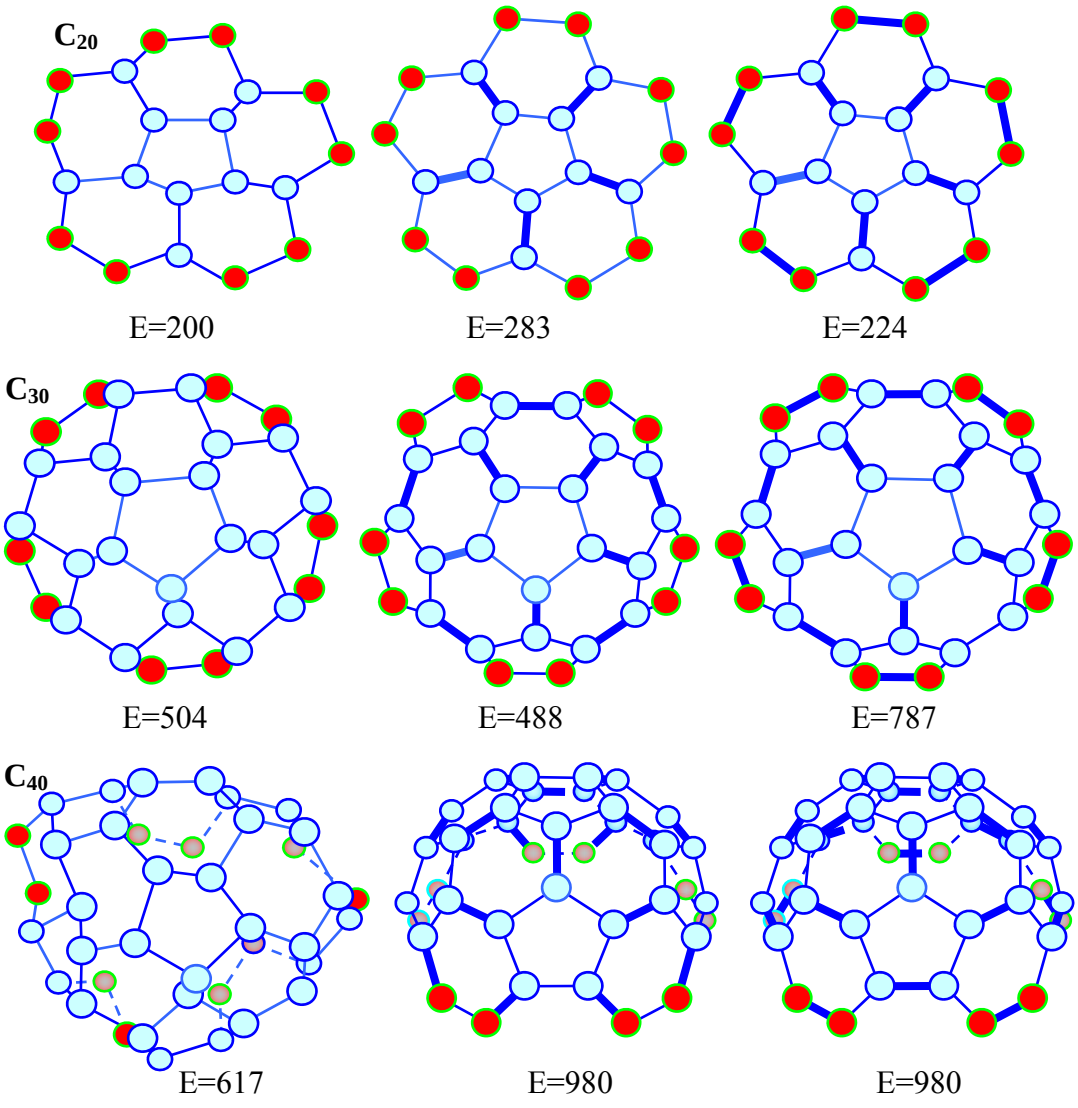



**Fig. 5**. Joining two dodecahedrons; structure and graphs; energy in kJ/mol

### 3. Cupolas and their fusion

Another way of looking at the gradual evolution of the clusters shown is the growth of initial clusters which then transform into half-fullerenes (cupolas) conserving the five-fold symmetry (Fig. 6). From the figures it is seen that all the cupolas have one and the same base of ten atoms; therefore they can combine with each other creating new fullerenes as well as nanotubes. Let us investigate this process in detail.



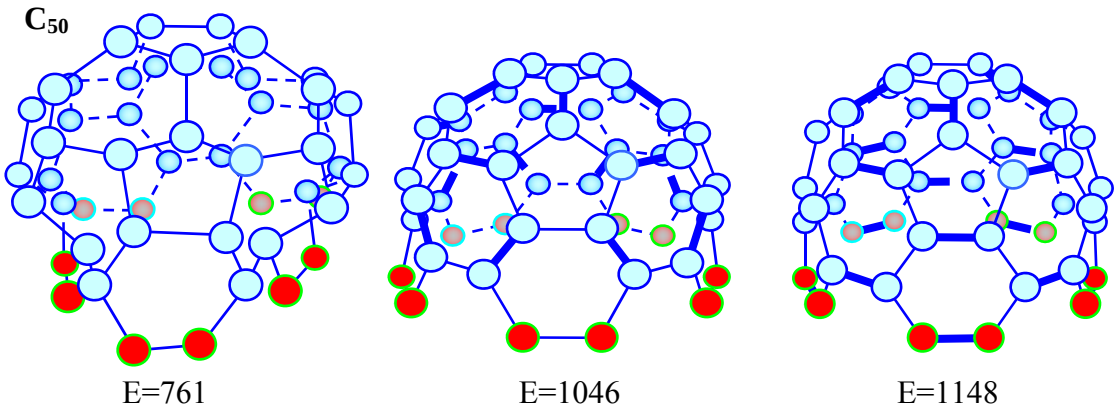



**Fig. 6.** Growth of cupolas of five-fold symmetry: structure and graphs; energy in kJ/mol

**Fusion of cluster $C_{10}$ with cupola $C_{20}$.** Here both initial configurations have five-fold symmetry. The fullerene obtained consists of five tetragons, two pentagons, and ten hexagons; it contains seventeen faces. One may name this perfect isomer, having five-fold symmetry, a truncated five-angular bipyramid (Fig. 7).

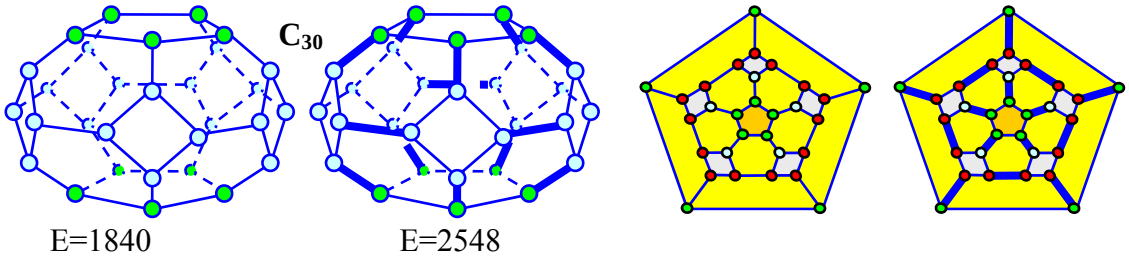



**Fig. 7.** Truncated five-angular bipyramid $C_{30}$ and its graphs; energy in kJ/mol

**Fusion of two cupolas $C_{20}$.** There are two ways of joining: mirror symmetry and rotation-reflection. In the first case (Fig. 8) the lower cupola is a mirror copy of the upper one. The fullerene obtained consists of five tetragons, two pentagons, and fifteen hexagons, and has twenty-two faces. In the second case (Fig. 9) the lower cupola is a rotatory reflection of the upper one. The fullerene obtained contains twelve pentagons and ten hexagons, the number of faces being the same. Its energy is less than that of the first fullerene.

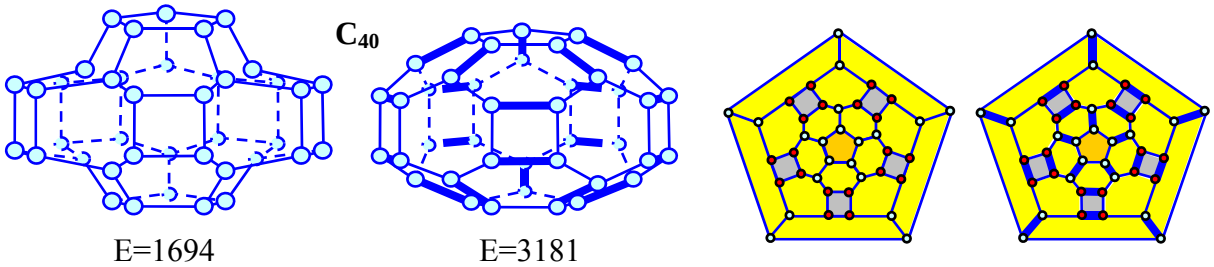



**Fig. 8.** Joining two cupolas $C_{20}$ of five-fold symmetry: the mirror symmetry fusion, structure and graphs; energy in kJ/mol

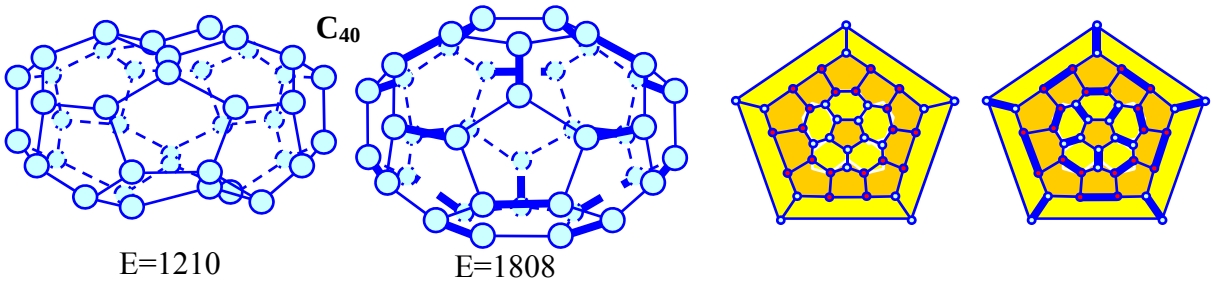



**Fig. 9.** Joining two cupolas $C_{20}$ of five-fold symmetry: the rotation-reflection symmetry fusion, structure, and graphs; energy in kJ/mol

**Fusion of two cupolas: $C_{20}$ and $C_{30}$** (Fig. 10). The atomic structure corresponding to a perfect polyhedron consists of two isolated pentagons, five sets of adjacent pentagons, and fifteen hexagons, so it can be named a penta$_{12}$-hexa$_{15}$ polyhedron.

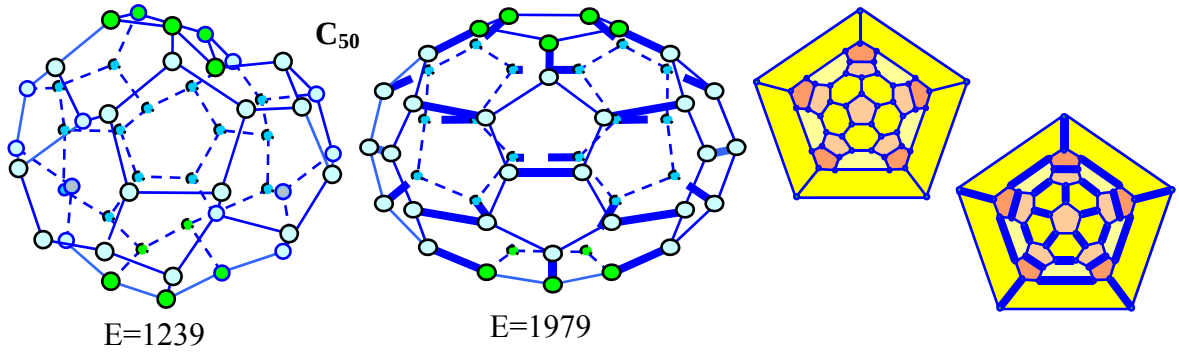



**Fig. 10.** Mirror symmetry fusion of two cupolas (half-fullerenes) $C_{20}$ and $C_{30}$ of five-fold symmetry; structure and graphs; energy in kJ/mol

**Fusion of two cupolas $C_{30}$** (Fig. 11). The atomic structure corresponding to a perfect polyhedron is a truncated icosahedron, which consists of twelve isolated pentagons and twenty adjacent hexagons. It is the most abundant and most celebrated fullerene molecule.

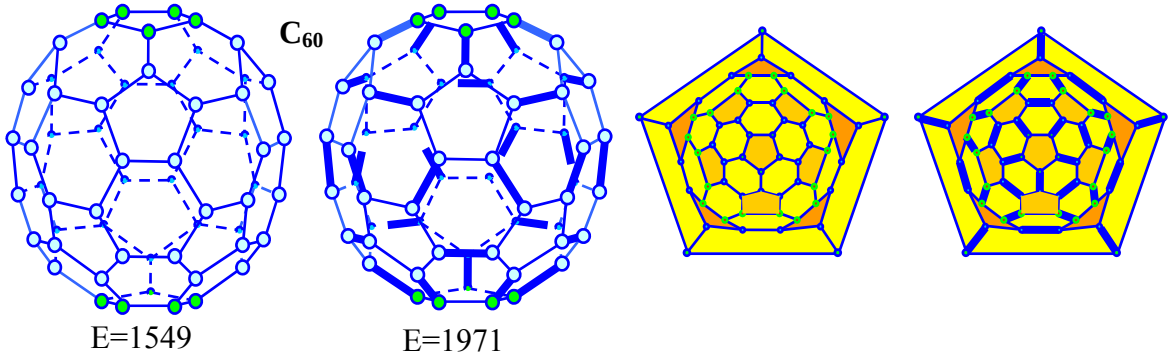



**Fig. 11**. Joining two cupolas $C_{30}$ of five-fold symmetry: the rotation-reflection symmetry fusion, structure, and graphs; energy in kJ/mol

**Fusion of two cupolas: $C_{30}$ and $C_{40}$** (Fig. 12). The atomic structure corresponding to a perfect polyhedron consists of twelve isolated pentagons, as before, and twenty-five adjacent hexagons. Beyond $C_{60}$, it is the next most abundant fullerene observed in the condensed carbon vapor.

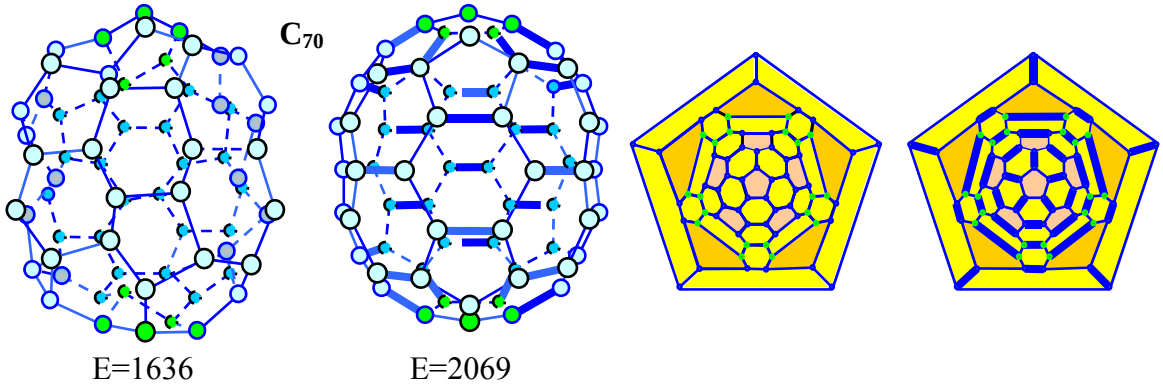



**Fig. 12.** Mirror symmetry fusion of two cupolas $C_{30}$ and $C_{40}$ of five-fold symmetry; structure and graphs; energy in kJ/mol

**Fusion of two cupolas $C_{40}$** (Fig. 13). It is a cigar-shaped molecule giving the beginning of the family of single-wall nanotubes (SWNT).

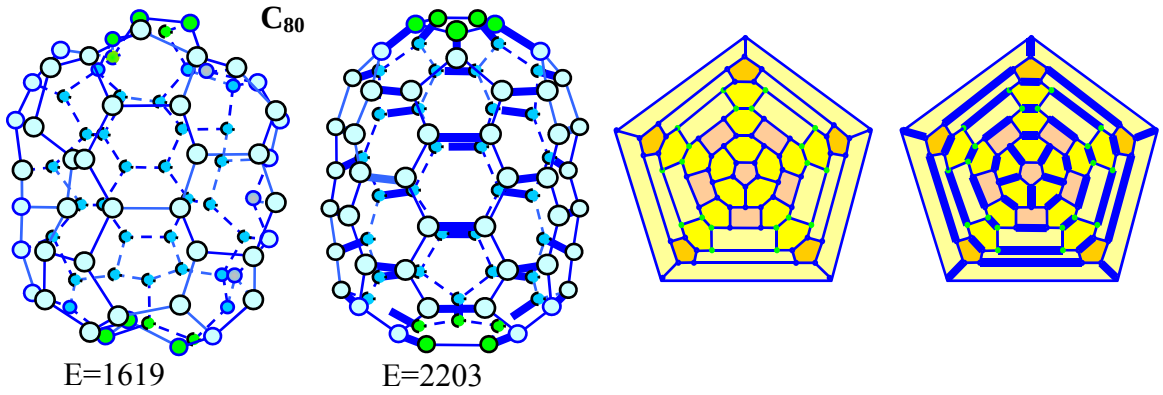



**Fig. 13.** Rotation-reflection-symmetry joining of two cupolas $C_{40}$ of five-fold symmetry; structure and graphs; energy in kJ/mol

**Fusion of two cupolas: $C_{40}$ and $C_{50}$**. The next in the column of five-fold symmetry is $C_{90}$, which atomic structure is shown in Fig. 14.

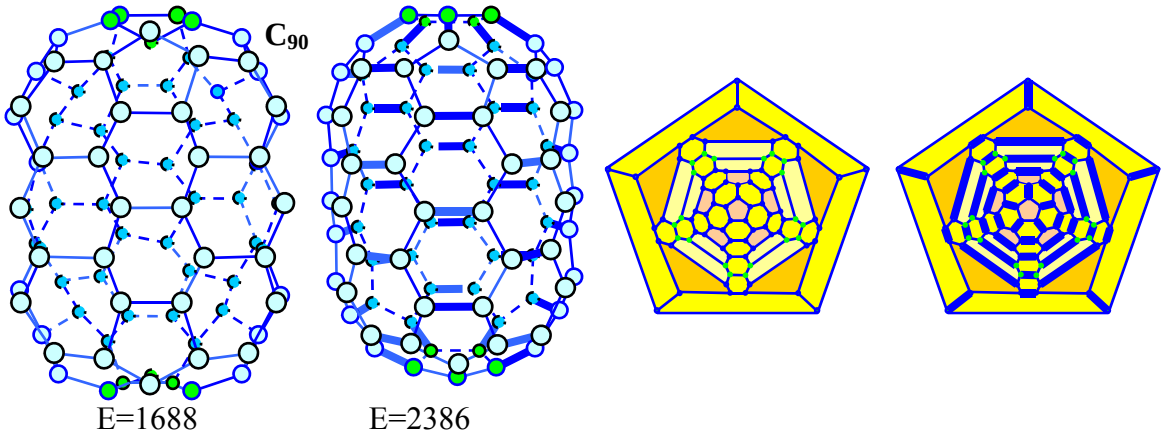


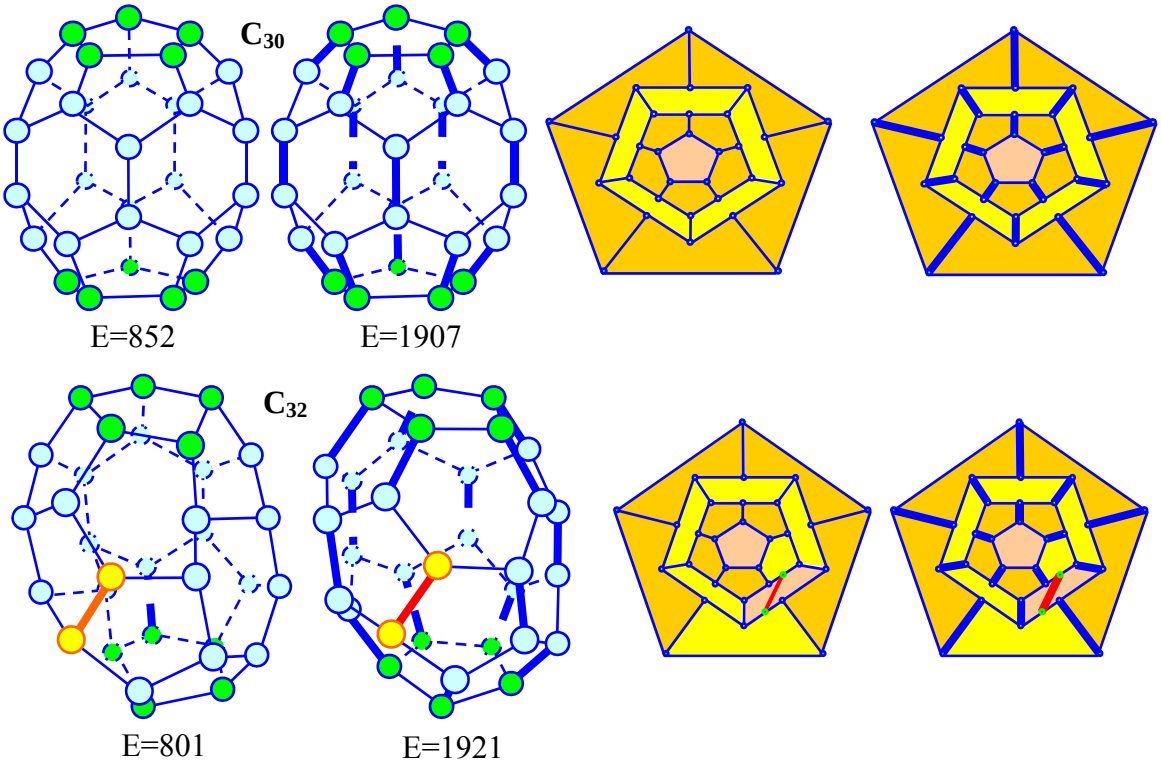

**Fig. 14.** Mirror symmetry fusion of two cupolas $C_{40}$ and $C_{50}$ of five-fold symmetry; structure and graphs; energy in kJ/mol

Let us analyze Figures 7-14. Hand in hand with different fullerenes of the five-fold symmetry, we have obtained two of the most abundant fullerene molecules $C_{60}$ and $C_{70}$ through the use of the cupola-fusion mechanism. Buckminsterfullerene $C_{60}$–$I_h$ is a truncated icosahedron [11]. This fullerene is considered an ideal one, having only equal isolated pentagons and forming a perfect sphere; each hexagon has three single and three double bonds. The measured bond lengths are $r_{hh}$ = 1.38 Å and $r_{hp}$ = 1.4654 Å. The larger bonds are singular, the lesser bonds are double ones. However, the formation mechanism, and especially the high yield of $C_{60}$–$I_h$ and $C_{70}$–$D_{5h}$, remains elusive and somewhat controversial.

In 2002 we have suggested and confirmed, through the use of molecular dynamics calculations, the fusion reaction mechanism of joining two hemispheres $C_{30}$ for obtaining fullerene $C_{60}$ [12]. This approach has succeeded in further development, at last leading to designing the periodic system of fullerenes [1,2]. According to the system, fullerene $C_{60}$ belongs to the Δn=12 series, the five-fold symmetry column, and has a lower formation energy than any of its nearest neighbors.

## 4. Intermediate fullerenes

**Growth of fullerene $C_{30}$.** The polyhedron shown in Fig. 4 can be thought of as a primary fullerene having the possibility to use for growing the mechanism known as "embedding carbon dimers" which was suggested by M. Endo and the Nobel Prize winner H.W. Kroto in 1992 [13]. According to it, a carbon dimer embeds into a hexagon of an initial fullerene. This leads to stretching and breaking the covalent bonds which are normal to the dimer and to create new bonds with the dimer. As a result, there arises a new atomic configuration and there is a mass increase of two carbon atoms. The fullerenes designed through the use of the Endo-Kroto mechanism are illustrated in Fig. 15.



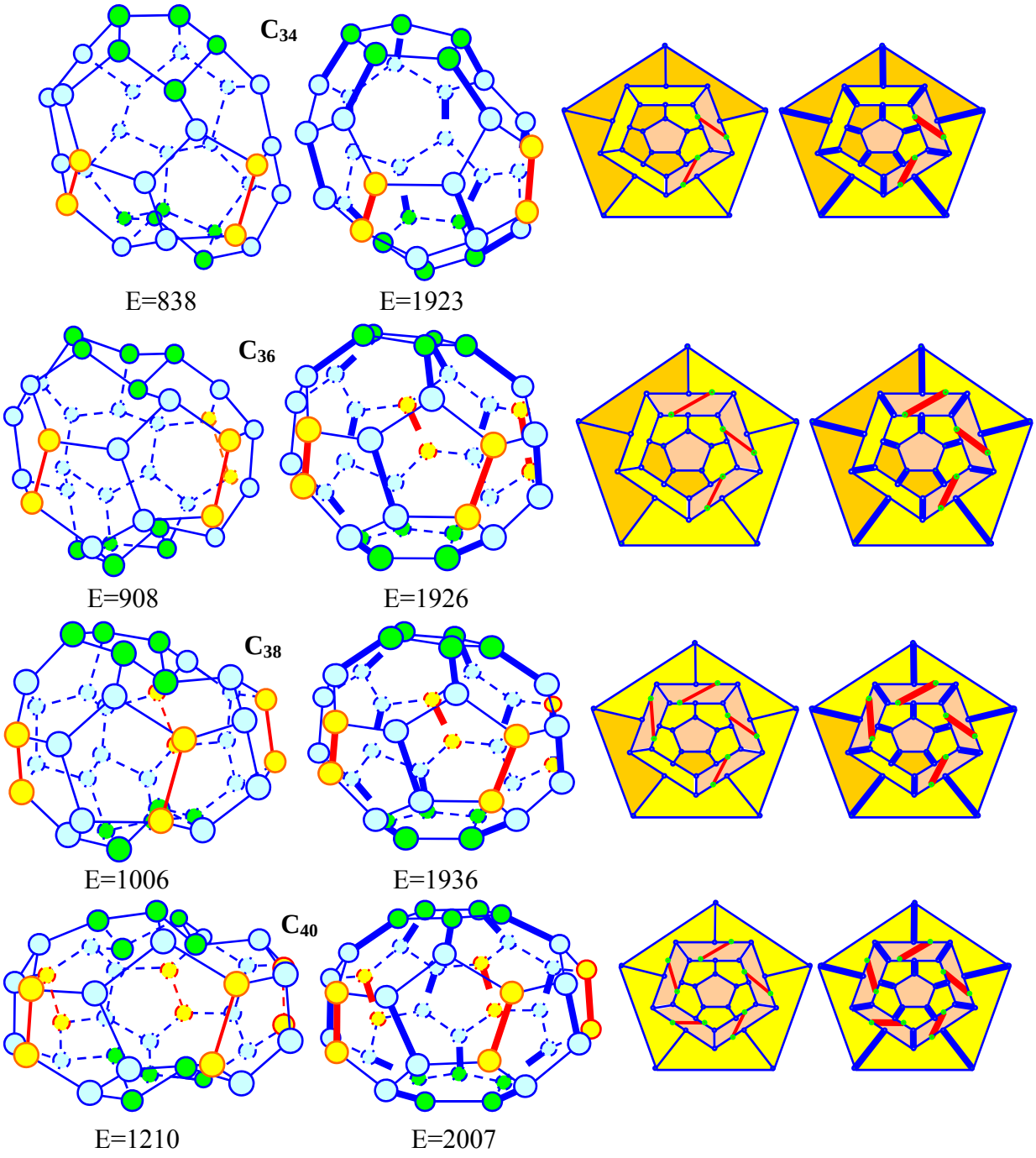
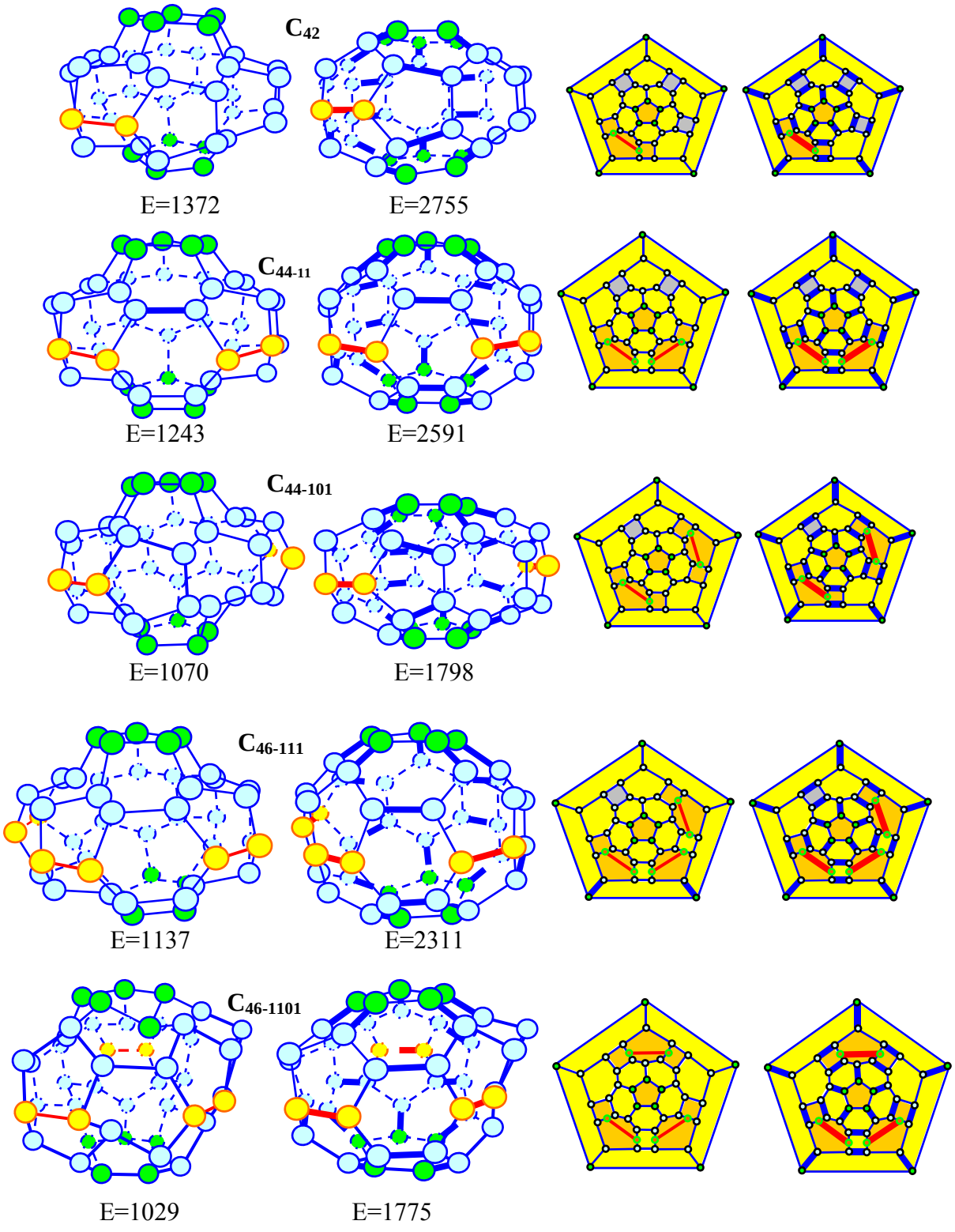



**Fig. 15.** Fullerenes $C_{32}$, $C_{34}$, $C_{36}$, $C_{38}$, and $C_{40}$ were obtained one after another by embedding a carbon dimer (yellow atoms) into fullerene $C_{30}$: structure and graphs; energy in kJ/mol

**Growth of fullerene $C_{40}$.**

*First cycle.* The fullerenes designed through the use of Endo-Kroto's mechanism of dimer embedding into a hexagon are illustrated in Fig. 16. Taking as a base the structure and graph of fullerene $C_{40}$, we have obtained the fullerenes from $C_{42}$ to $C_{50}$ one after another embedding a carbon dimer (yellow atoms) into fullerene $C_{40}$.


C42
E=1372
E=2755
C44-11
E=1243
E=2591
C44-101
E=1070
E=1798
C46-111
E=1137
E=2311
C46-1101
E=1029
E=1775

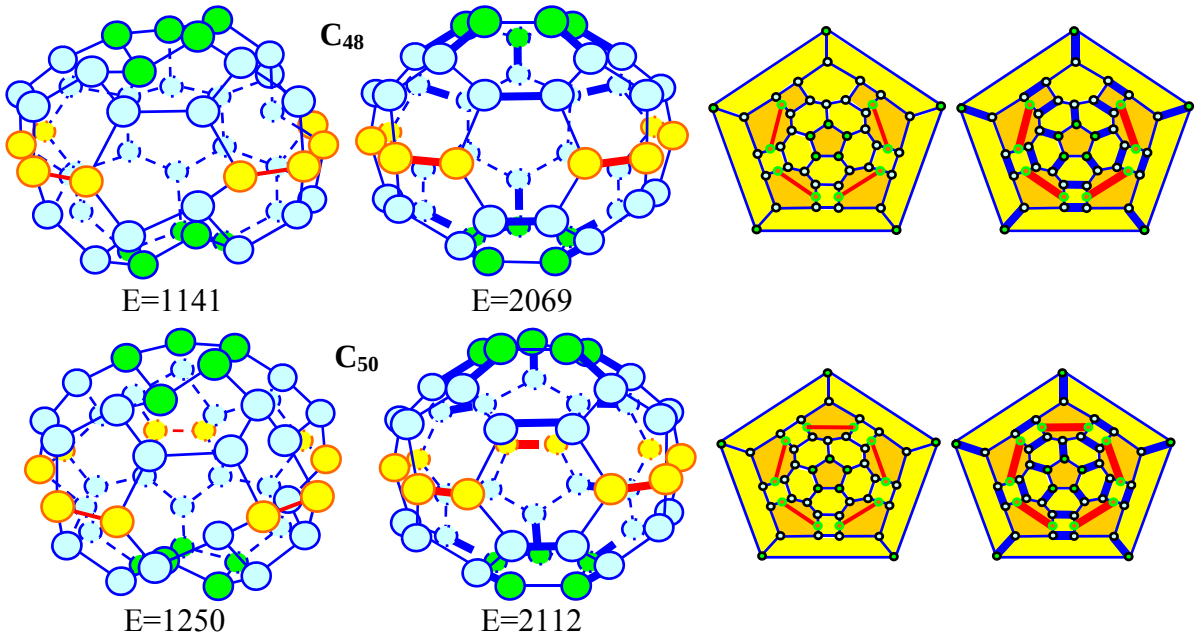



**Fig. 16.** Fullerenes $C_{42}$, $C_{44}$, $C_{46}$, $C_{48}$, and $C_{50}$ were obtained one after another by embedding a carbon dimer (yellow atoms) into fullerene $C_{40}$: structure and graphs; energy in kJ/mol

From the figure, it follows that only the initial and final fullerenes $C_{40}$ and $C_{50}$ have ordinary five-fold symmetry. They are perfect fullerenes. The intermediate fullerenes from $C_{42}$ to $C_{48}$ have topological five-fold symmetry. Among the intermediate fullerenes, there are two isomers of fullerene $C_{44}$ and two isomers of fullerene $C_{46}$ having one and the same topological symmetry but different shapes. The shape difference is connected with the diverse location of embedded dimers at the equator. These fullerenes obtained will be named permutation isomers and be denoted as 11 and 101, and as 111 and 1101. Indices 11 and 111 indicate that the embedded dimers are the nearest (first) neighbors; indices 101 and 1101 point to the fact that two dimers are the second neighbors. It is worth noting that the energy of fullerenes is less in the second case. To gain a better understanding of the mechanism of dimer embedding, its main features are shown schematically in Fig. 17.

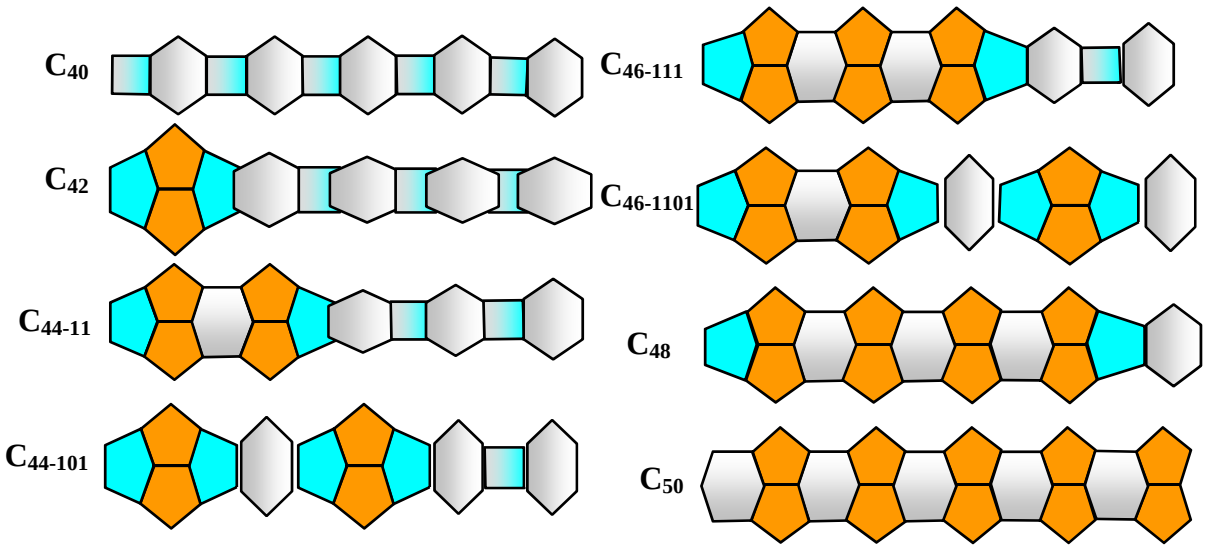
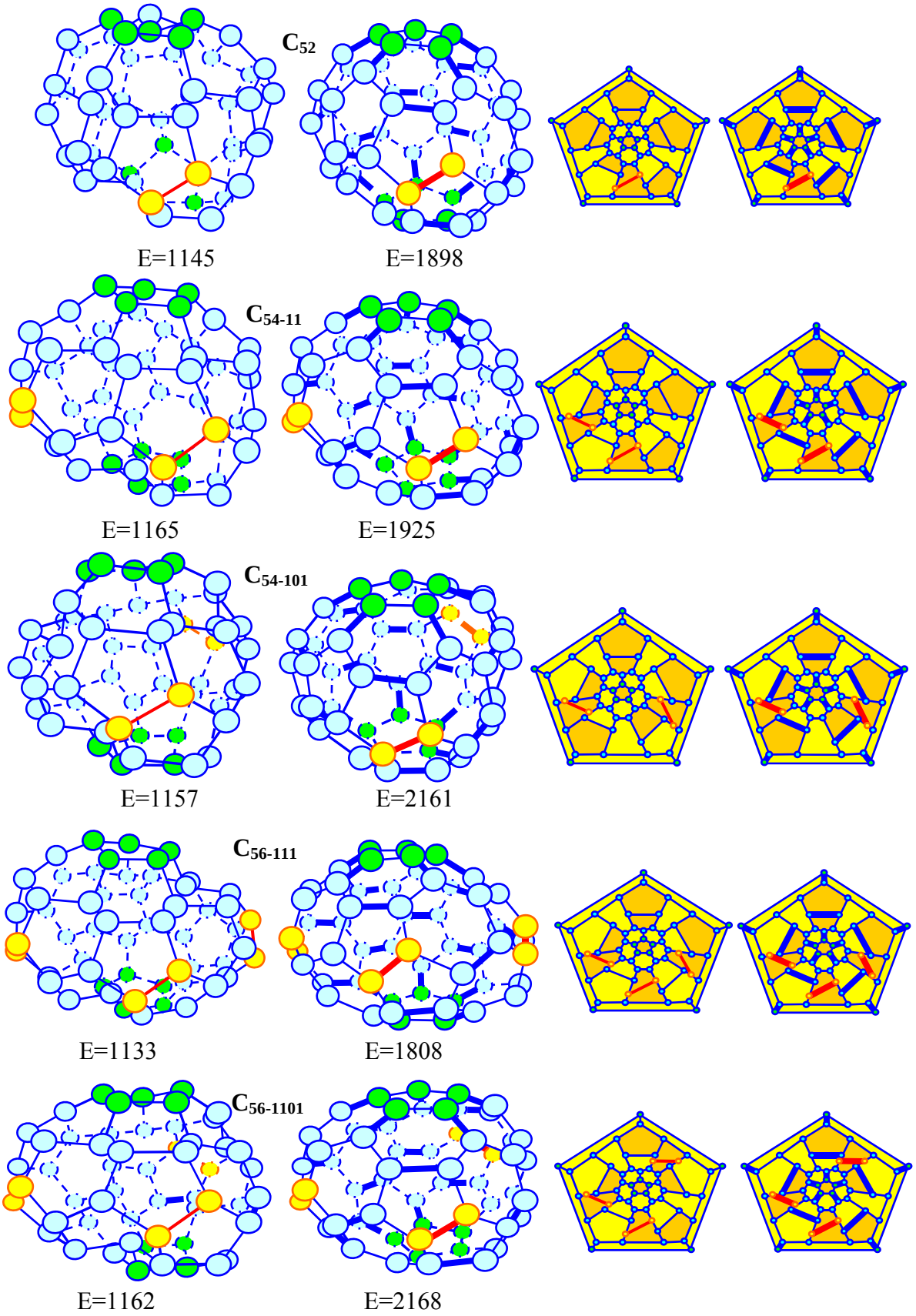



**Fig. 17.** Scheme of the main structural changes during the first stage growth of fullerene $C_{40}$

*Second cycle*. The growth can continue producing imperfect fullerenes from $C_{52}$ to $C_{58}$ and perfect fullerene $C_{60}$ (Fig. 18). To gain a better understanding of the process, its main features are given in the form of schematic representation (Fig. 19).



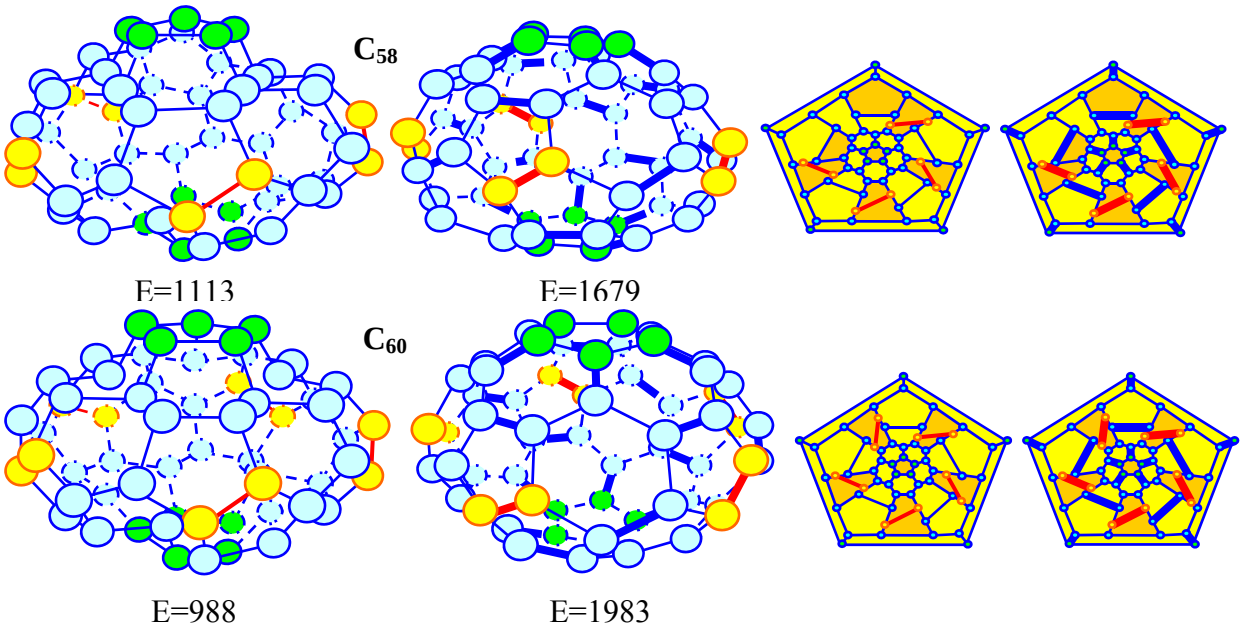



**Fig. 18.** Fullerenes $C_{52}$, $C_{54}$, $C_{56}$, $C_{58}$, and $C_{60}$ obtained by one-after-another embedding a carbon dimer (yellow atoms) into fullerene $C_{50}$: structure and graphs; energy in kJ/mol

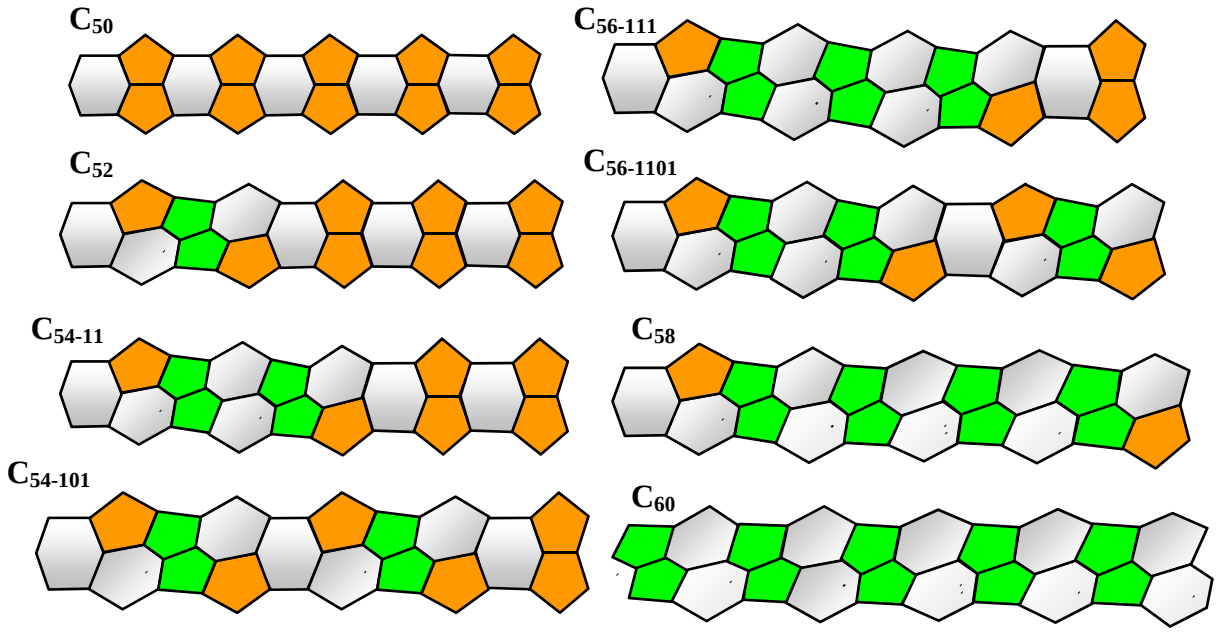
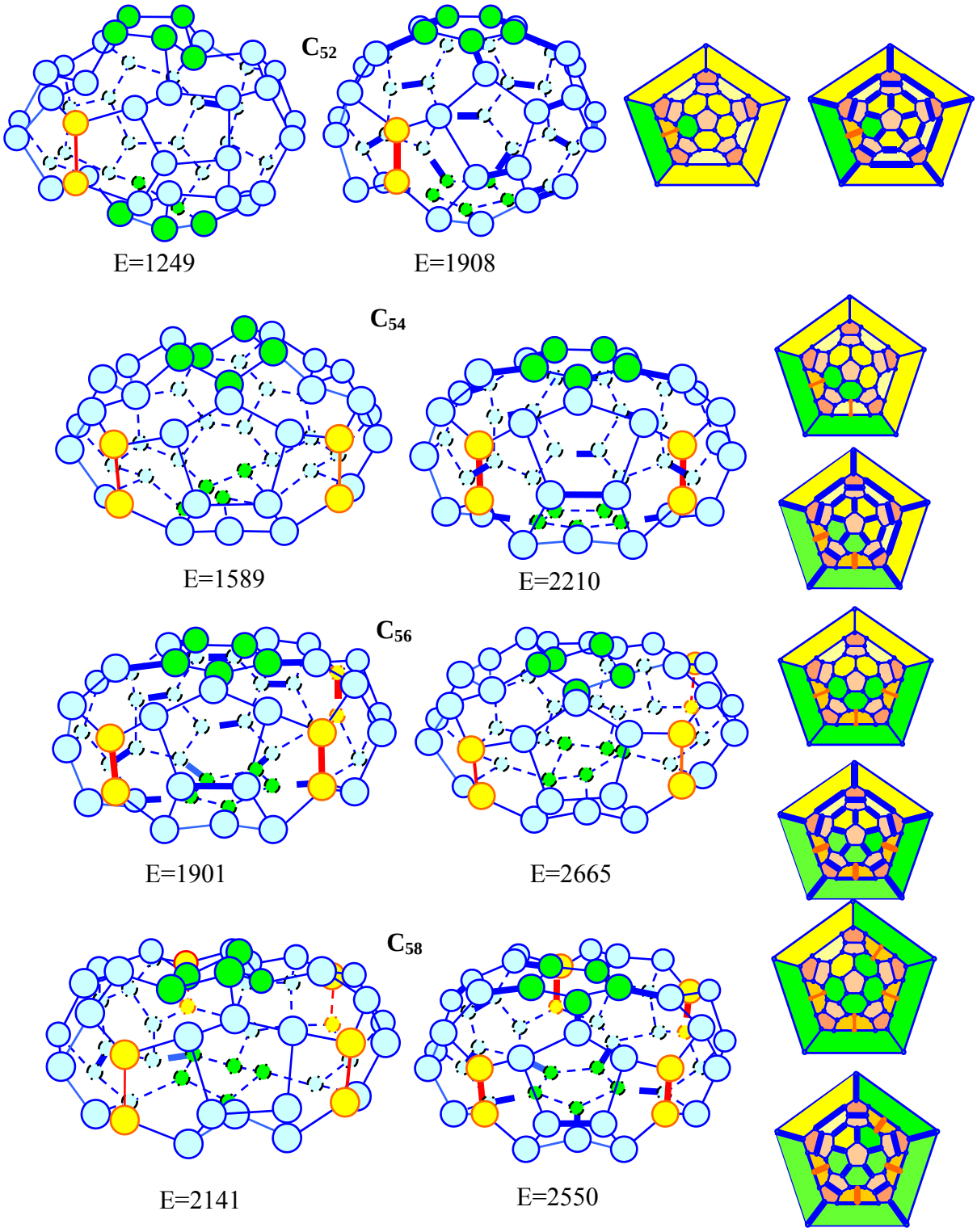



**Fig. 19.** Scheme of the main structural changes during the first stage growth of fullerene $C_{40}$

We see that fullerene $C_{50}$ can grow by embedding the dimers only at an angle to its main axis of symmetry; it follows from Figs. 18 and 19. The phenomenon is connected with the fact that embedding can be realized only normally in a direction along which a hexagon has two neighboring mutually antithetic pentagons. During further growth, one obtains fullerenes $C_{52}$, $C_{54}$, $C_{56}$, $C_{58}$, and $C_{60}$. Similar to the first cycle, the intermediate fullerenes are imperfect, but fullerene $C_{60}$ having five embedded dimers is perfect. It should be emphasized that in this case, the number of embedded dimers is equal to the degree of symmetry. It should be emphasized that this fullerene differs from that obtained by the fusion of cupolas (Fig. 11).

**Growth of fullerene $C_{50}$ (Non-classical fullerenes)**. The growth of fullerene $C_{50}$ can continue in another way producing also imperfect fullerenes $C_{52}$, $C_{54}$, $C_{56}$, $C_{58}$, and perfect fullerene $C_{60}$ (Fig. 20). The fullerenes are obtained as a result of embedding one after another carbon dimer into fullerene $C_{50}$ parallel to the five-fold axis. From the figures, we notice again that only the initial and final fullerenes $C_{50}$ and $C_{60}$ have ordinary five-fold symmetry. They are perfect fullerenes. The intermediate fullerenes $C_{52}$, $C_{54}$, $C_{56}$, and $C_{58}$ have topological five-fold symmetry.



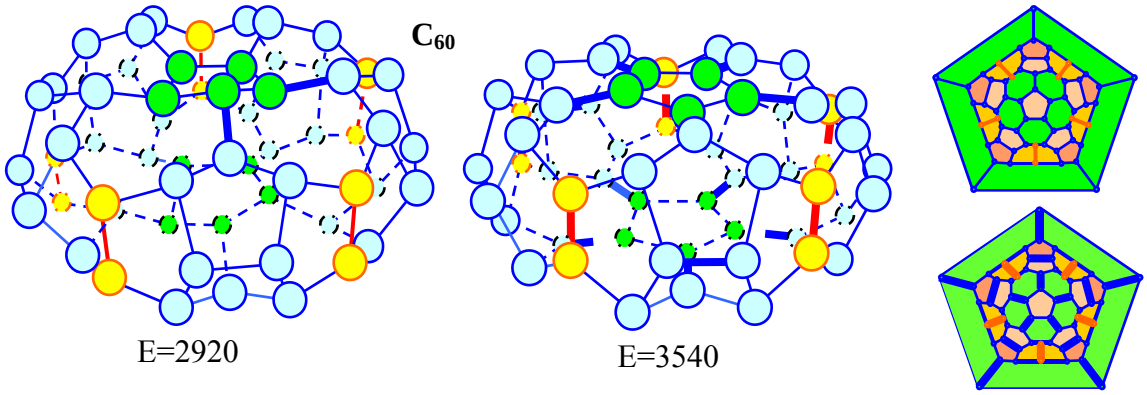
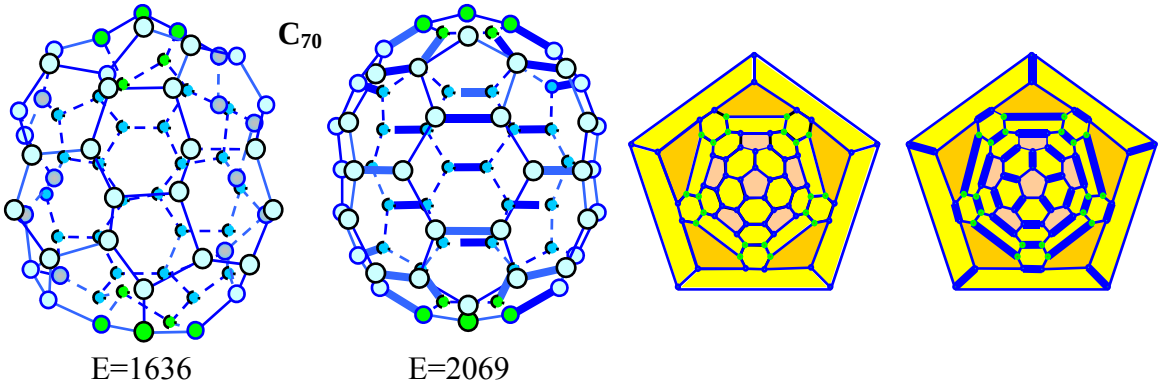


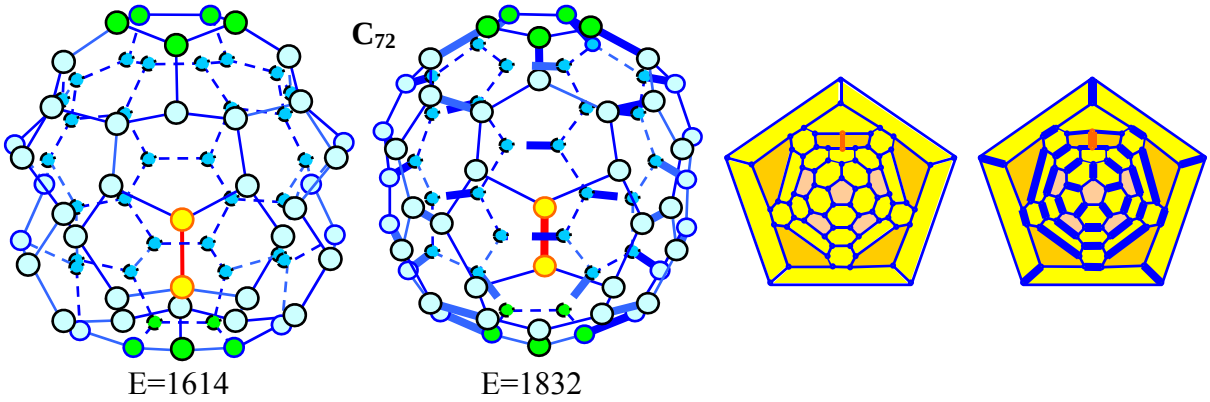

**Fig. 20.** Fullerenes $C_{52}$, $C_{54}$, $C_{56}$, $C_{58}$, $C_{60}$ were obtained one-after-another embedding a carbon dimer into fullerene $C_{50}$ parallel to the five-fold axis: structure and graphs; energy in kJ/mol

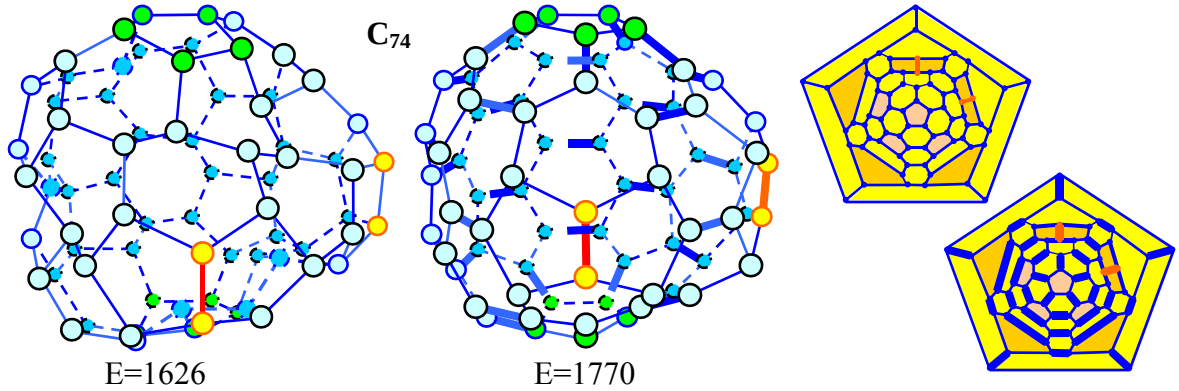
These results deserve further comment. For a detailed discussion of this subject see [10]. According to the authors, "In general, classical fullerenes are cage-like, hollow molecules of pseudospherical symmetry consisting of pentagons and hexagons *only*, resulting in a trivalent (and in the most ideal case) convex polyhedron with exactly three edges (bonds) joining every vertex occupied by carbon, idealized as $sp^2$ hybridized atoms. What happens if we relax the rules a little bit, and allow for other types of three-valent ($sp^2$) carbon framework? There are many generalizations that lead to structures of beautiful shapes that have both elegant mathematical theory and physical realizations: allowing for polygons with faces different from pentagons and hexagons. What kinds of fulleroids, which are fullerene-like structure, are allowed? Can we tile a sphere or a torus with heptagons only, or with only pentagons and heptagons?" Figure 20 answers the questions.

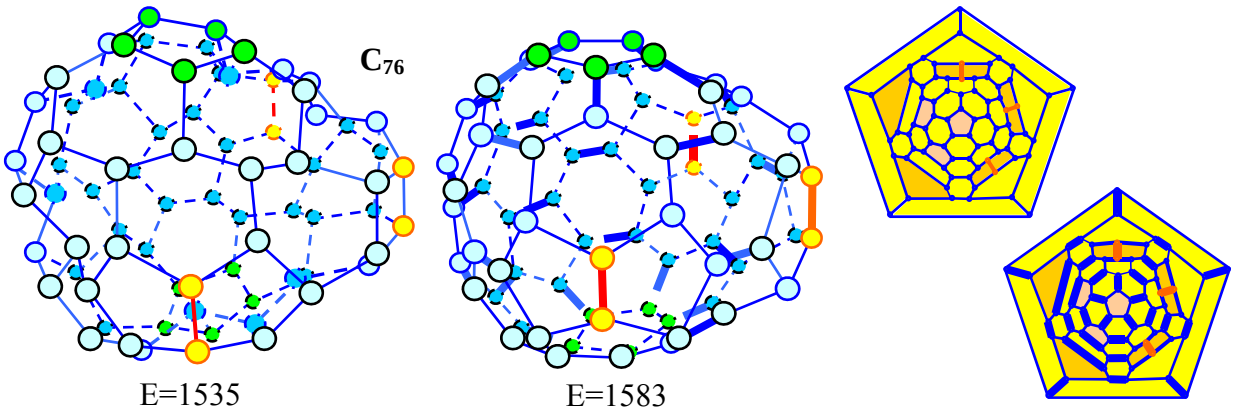
From the configurations shown it follows that the first embedding, which transforms fullerene $C_{50}$ into fullerene $C_{52}$, influences deeply only one of the hexagons and two of its hexagon neighbours. This hexagon transforms into two adjacent pentagons and its hexagon neighbors become heptagons; the fullerene $C_{52}$ losing ordinary five-fold symmetry. It becomes an imperfect fullerene with the ordinary $D_{1h}$ symmetry, however conserving topological five-fold symmetry. At that in the fullerene, there appears a cell that contains four pentagons. The second embedding transforms fullerene $C_{52}$ into fullerene $C_{54}$. The third embedding leads to transition from fullerene $C_{54}$ to fullerene $C_{56}$. It transforms one more hexagon and two of its neighbors into two adjacent pentagons with about heptagons. The fourth embedding acts in a similar manner. At last, the fifth embedding restores $D_{5h}$ symmetry. The perfect fullerene $C_{60}$ obtained contains only pentagons (22) and heptagons (10), and no hexagons. It is a $penta_{22}$-$hepta_{10}$ polyhedron; its shape resembles more a disk than a spheroid.

**Growth of fullerene $C_{70}$.** The fullerene belongs to the column of basic perfect fullerenes having five-fold symmetry. It can produce the natural isomers shown in Fig. 21.


C70
E=1636
E=2069


C72
E=1614
E=1832


C74
E=1626
E=1770


C76
E=1535
E=1583

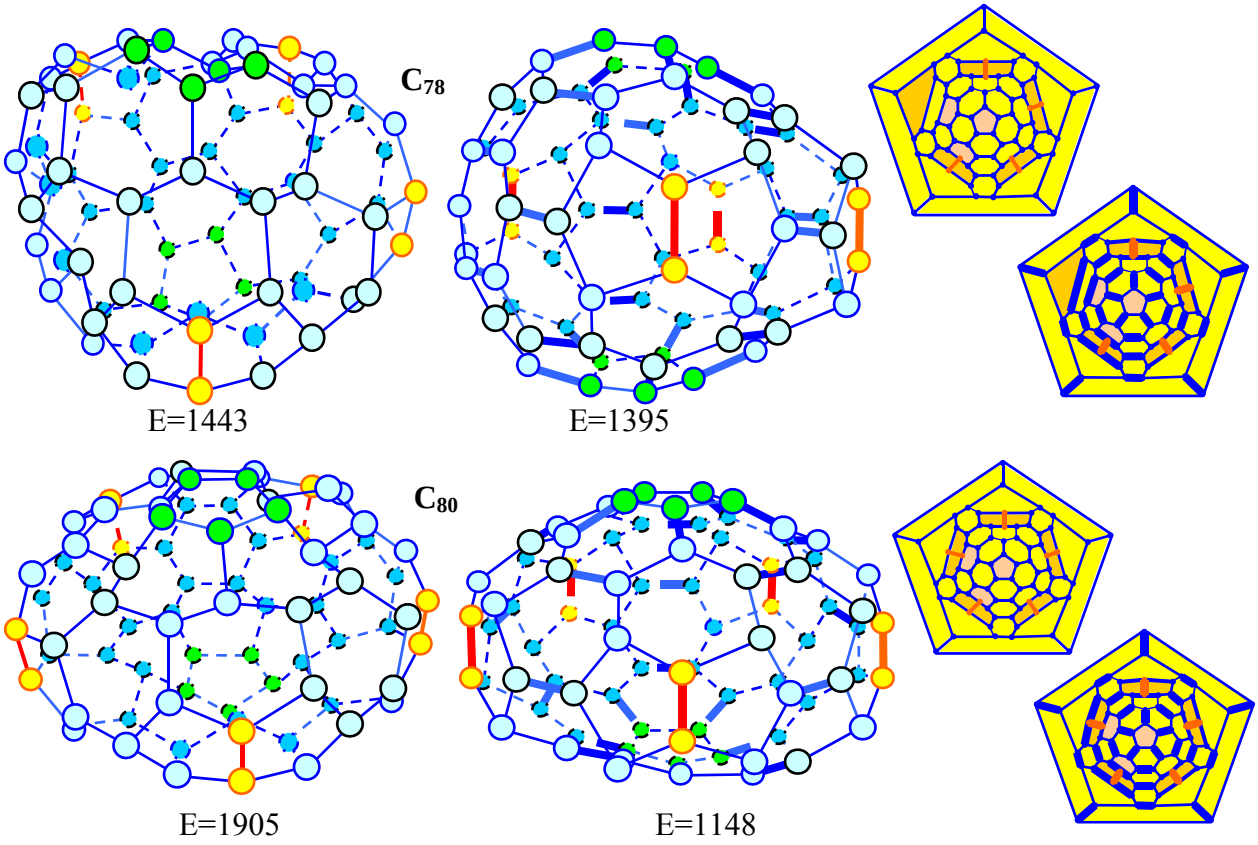
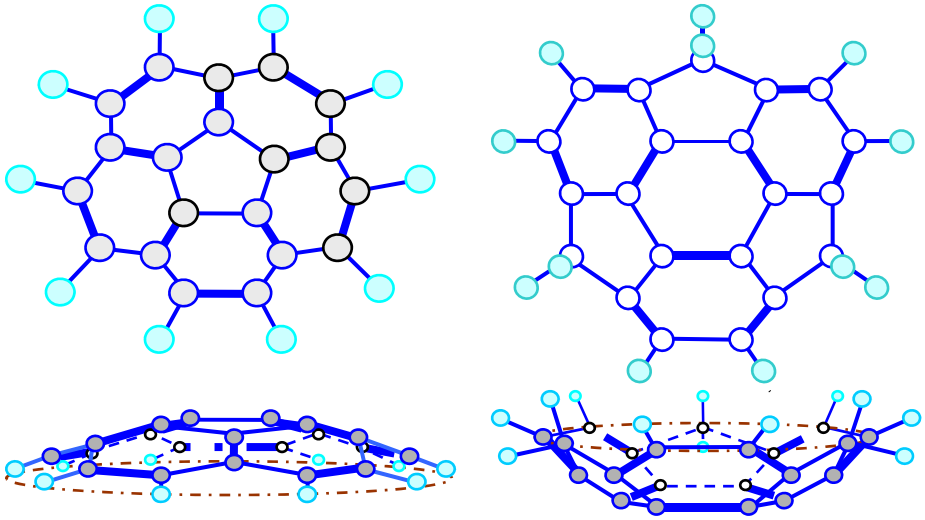



**Fig. 21.** Fullerenes $C_{58}$, $C_{60}$, $C_{62}$, and $C_{64}$ as a result of one-after-another carbon dimer embedding into fullerene $C_{56}$: structure and graphs; energy in kJ/mol

## 5. Corannulene, sumanene and fullerene $C_{60}$

We have designed the most abundant and most celebrated fullerene molecule $C_{60}$ by fusion of two cupolas $C_{30}$ (Fig. 11). The atomic structure corresponding to a perfect polyhedron is a truncated icosahedron, which consists of twelve isolated pentagons and twenty adjacent hexagons. It should be emphasized that the formation and structure of cupolas were postulated. The question arises: Are there in nature similar molecules, from which it is possible to obtain the cupolas? To our mind corannulene $C_{20}H_{10}$ with $C_{5v}$ symmetry and sumanene $C_{21}H_{12}$, which possesses $C_{3v}$ symmetry, could be such molecules. These molecules are usually considered key fullerene fragments [14,15]. Being π-conjugated compounds, they are bowl-shaped or cupola-shaped species; it depends on a point of view (Fig. 22). The bowl of sumanene (1.15 Å) is anticipated to be deeper than that of corannulene (0.89 Å). According to [13], deeper π-bowls are more interesting because they may have properties more similar to those of fullerenes.

Early we investigated the possible ways of fullerene obtained from sumanene [16]. Now discuss the role of corannulene and compare it with those of sumanene. Suppose that we have removed ten hydrogen atoms from corannulene, then we obtain cupola $C_{20}$. If afterward add ten carbon atoms to the cupola, one gets cupola $C_{30}$ (Fig. 23). The fusion of two cupolas leads to the appearance of the most famous fullerene molecule $C_{60}$ (Fig. 24). To gain a better understanding of the fusion reactions, their main features are given in the form of a scheme (Fig. 25).



Corannulene $C_{20}H_{10}$ Sumanene $C_{21}H_{12}$

**Fig. 22.** Corannulene as a cupola and sumanene as a bowl (energy, kJ/mol)

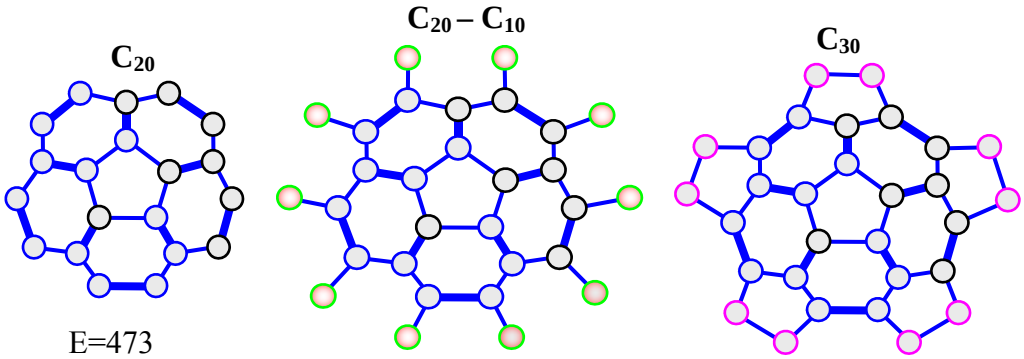



**Fig. 23.** Carbon cupolas generated on the basis of corannulene: energy in kJ/mol

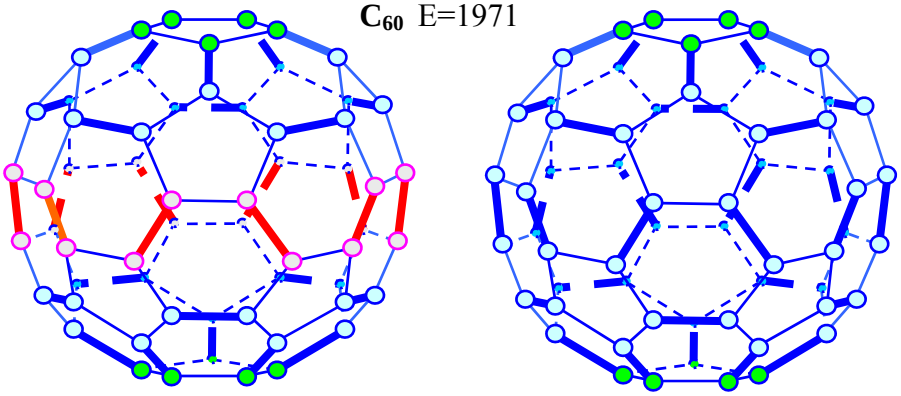



**Fig. 24.** Fullerene $C_{60}$ was obtained by the fusion of two corannulene cupolas $C_{30}$: energy in kJ/mol

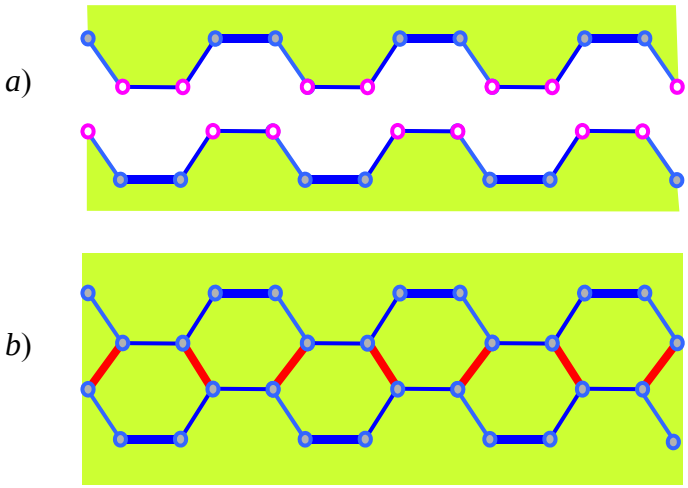



**Fig. 25.** Scheme reflecting the main structural changes during the fusion of cupolas: a) boundary-atom configuration of separate cupolas; b) fusion zone

In a similar manner it is possible to obtain from sumanene successively cupolas $C_{21}$ and $C_{30}$ and afterward fullerene $C_{60}$ (Figs. 26 and 27). Interestingly enough that the final structures of the fullerenes obtained in different ways are the same. However, in the second case, there are possible fusion faults (Figs. 28 and 29).

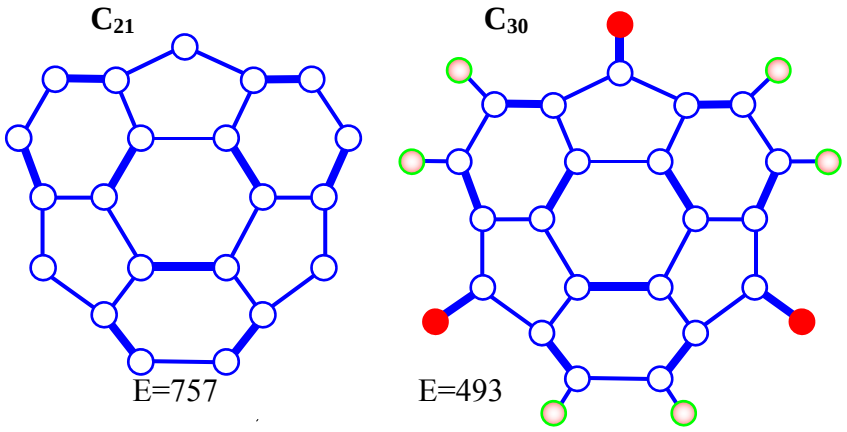



**Fig. 26.** Carbon cupolas generated on the basis of sumanene: energy in kJ/mol

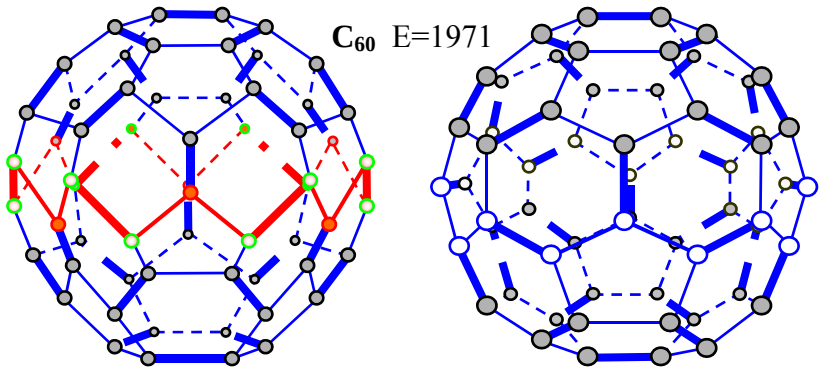



**Fig. 27.** Fullerene $C_{60}$ was obtained by the fusion of two sumanene cupolas $C_{30}$: energy in kJ/mol

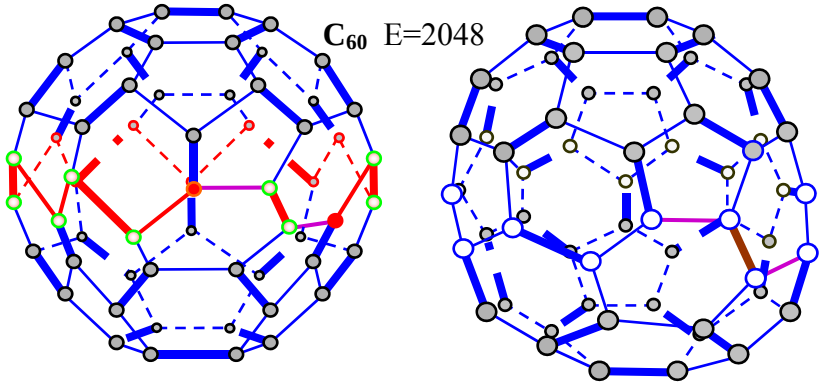



**Fig. 28.** Fullerene $C_{60}$ was obtained by the fault-fusion of sumanene cupolas $C_{30}$: energy in kJ/mol

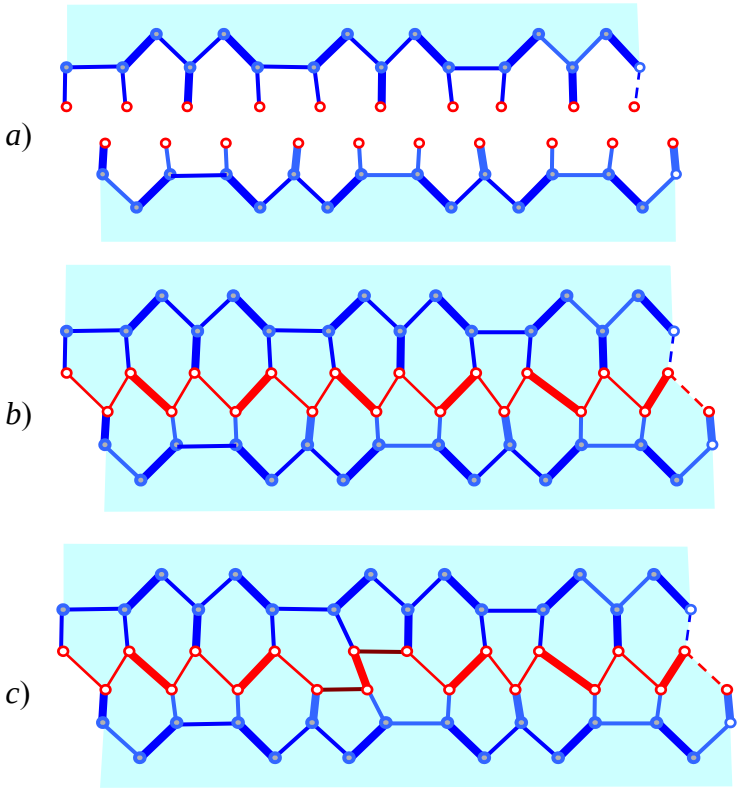



**Fig. 29.** Scheme reflecting the main structural changes during the fusion of cupolas: a) boundary-atom configuration of separate cupolas; b) fusion zone, perfect reaction; c) fusion zone, fault one

These results deserve further comment. The mechanism of fusion resembles that known in biophysics as lock-key adhesion [17]. The adhesion is due to the formation of specific molecular bonds between complementary pairs of proteins which are denoted by "lock" (L) and "key" (K). In our case, the boundary-atom configurations of cupolas play simultaneously the role of both lock and key. For the corannulene cupolas, the LK atoms are rather rigidly connected with the whole cupolas by two interatomic bonds; it follows from Fig. 25a. On contrary, for the sumanene cupolas thermal fluctuations are more important for the LK atoms since these atoms are connected with the cupolas only by one bond, single or double, (Fig. 29a). As a result, the "sumanene" fullerenes can contain fusion faults (Fig. 29c).

## 6. Conclusion

We have studied possible ways of generating and growing the fullerenes having five-fold symmetry. Beginning with cyclopentane $C_5H_{10}$ and clusters $C_5C_5$, we obtained at first elementary fullerenes $C_{10}$ and mini-fullerenes $C_{20}$, and then the fullerenes from $C_{30}$ to $C_{80}$, perfect and imperfect, as well as nanotubes. The imperfection is connected either with extra 'interstitial' carbon dimers, the dimers playing the role of defects. Only the basic fullerenes $C_{30}$, $C_{40}$, $C_{50}$, $C_{60}$, $C_{70}$, and $C_{80}$ have the ordinary five-fold symmetry in the corresponding column of the periodic system of fullerenes, the intermediate fullerenes having no such symmetry. Considering the latter as imperfect due to defects, one can define them as the fullerenes conserving *topological* five-fold symmetry. We have calculated the energies of the possible fullerenes.

We have designed the most abundant and most celebrated fullerene molecule $C_{60}$ by fusion of two cupolas $C_{30}$. The atomic structure corresponding to a perfect polyhedron is a truncated icosahedron, which consists of twelve isolated pentagons and twenty adjacent hexagons. It should be emphasized that the formation and structure of cupolas were postulated. The question arises: Are there in nature similar molecules, from which it is possible to obtain the cupolas? To our mind corannulene $C_{20}H_{10}$ with $C_{5v}$ symmetry and sumanene $C_{21}H_{12}$, which possesses $C_{3v}$ symmetry, could be such molecules. These molecules are usually considered key fullerene fragments. Being π-conjugated compounds, they are bowl-shaped or cupola-shaped species. The mechanism of fusion resembles that known in biophysics as lock-key adhesion. The adhesion is due to the formation of specific molecular bonds between complementary pairs of proteins which are denoted by "lock" (L) and "key" (K). In our case, the boundary-atom configurations of cupolas play simultaneously the role of both lock and key. For the corannulene cupolas, the LK atoms are rather rigidly connected with the whole cupolas by two interatomic bonds. On contrary, for the sumanene cupolas, thermal fluctuations are more important for the LK atoms since these atoms are connected with the cupolas only by one bond (single or double). As a result, the "sumanene" fullerenes can contain fusion faults.

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