Materials Physics and Mechanics 34 (2017) 1-17 Received: October 3, 2017

UNIFIED APPROACH TO FORMING FULLERENES AND NANOTUBES

Alexander I. Melker[1*] and Maria A. Krupina[2]

[1] Department of Mechanics and Control Processes,

[2] Department of Experimental Physics,

Peter the Great St. Petersburg Polytechnic University, Polytekhnicheskaya 29

195251, St. Petersburg, Russia

*e-mail: newton@imop.spbstu.ru

Abstract. Reactions of elementary fullerenes (from C_4 to C_{12}) with each other as well as with their heirs are considered. Under the elementary fullerenes we understand a tetrahedron, a cube, and triangular, pentagonal and hexagonal prisms. The process is similar to fusion of bubbles in a soap solution. The graphs describing the process are suggested. The reaction zone is a vertex-connected subgraph that takes into account physical restrictions, namely that covalent bonds exist only between nearest-neighbor atoms. We supposed that during the reactions new covalent bonds are formed and old covalent bonds between the reacting atoms are destroyed. The clusters obtained resemble both fullerenes and nanotubes.

Keywords: fullerene, fusion, graph, growth, nanotube.

1. Introduction

Discoveries and consequences. Since the discovery of fullerenes [1, 2], carbon nanotubes [3], and graphene [4, 5] carbon occupies a strategic position in materials science and technology as one of the most versatile and far-reaching materials [6-17]. Two small fullerenes have been detected with the mass spectroscopic method, C_{36} [18] and C_{20} [19]. The synthesis and separation of molecules C_{36} from arc derived carbon has attracted considerable attention, since fullerenes smaller than C_{60} are highly strained due to the presence of fused five-membered rings. Caged molecules with low mass in the fullerene family are especially interesting because of their high curvature and increased strain energy that give rise to high reactivity.

Small fullerenes. Current studies on fullerenes and their compounds focus on large-size fullerenes mainly. Systematic studies on small (middle-size) fullerenes and non-isolated-pentagon-ring (IPR) fullerenes are less common. The structure and stability of fullerenes containing less than 60 carbon atoms have been studied experimentally and theoretically [17-70]. Experimental researches of such fullerenes are still limited by low yield and poor stability. As a result, theoretical methods prevail. Only works [18, 19, 21, 33, 56, 57, 60, 65, and 67] refer to experimental investigations. Endohedral metallofullerenes MC_{28} were obtained in Ref. [57] where M=Ti, Zr, U. In Ref. [33] decachlorfullerene $C_{50}Cl_{10}$ was synthesized.

The most comprehensive experimental study [60] revealed the following. (We conserve here the terminology by the authors). In the mass spectra of products of benzene pyrolysis, the authors found out the ions of all kinds of carbon molecules including *a)* small carbon molecules (C_3-C_{20}); *b)* quasi-fullerenes C_{21}, C_{23}, C_{33}, C_{48}, C_{52}, C_{54}, C_{56} and C_{58}; *c)* hydrides of small carbon molecules, C_5H_2, $C_{10}H_4$, $C_{14}H_4$, $C_{16}H_8$ and $C_{18}H_2$, *d)* hydrides of quasi-fullerenes: $C_{25}H_2$, $C_{27}H_2$, $C_{31}H_4$, $C_{37}H_6$, $C_{39}H_6$, $C_{43}H_8$, $C_{47}H_{10}$ and $C_{49}H_{10}$. In the authors' opinion [60] the absence of

appreciable progress in synthesis C_n (n<20) and quasi-fullerenes is determined by the domination of hypothesis that carbon atoms are always necessary for growth of carbon molecules; their generating being possible only under carbon sublimation.

The theoretical methods are helpful in this field to discover some potential compounds with good properties. The most of them refer to searching criteria on the stability of fullerene molecules having different structures. This is an important task because the influence of fullerene structure on their stability and properties is crucial. We will not analyze the methods used by the authors since they have both advantages and drawbacks. "Carbon, however, appears able to break so many rules that one must continually reconsider them for this element. It is, after all, only after a great deal of study that the structures of even the smallest molecules such as C_2 and C_3 have been characterized and understood theoretically. Such studies urge caution in being too hasty with regards to assumptions about the electronic and geometric structure of carbon compounds in terms of conventional valence theory" wrote Harold W. Kroto who shared the 1996 Nobel Prize for chemistry for his co-discovery of fullerenes [2]. We consider the theoretical studies from the point of view of the aims that their authors set themselves. On this basis the theoretical investigations can be divided into several groups.

1) The authors studied well-established experimentally fullerenes; their properties, the stability of their isomers, and the interactions with other molecules [24, 25, 32, 46, 52, 54, 62].

2) The authors studied the stability of different isomers of one and the same fullerene. The isomer structures are chosen from a lot of postulated combinatorial ones [53, 68 and 70].

3) The authors tried to fulfill the gap between the fullerenes found experimentally and those that could be synthesized. The structure of theoretically possible fullerenes was also postulated [20, 22, 23, 28, 29, 31, 35-39, 43, 44, 47-51, 66, 69].

It must be emphasized that most investigations of small fullerenes have centered on either obtaining these materials experimentally or theoretical studying properties of these materials which structure was usually postulated. To our mind, the crucial questions for advanced applications of all the fullerenes are: how the materials are originated and what structure they obtain. Answer to these questions gives the possibility to develop nanotechnology on a scientific basis.

Nucleation and growth. Up to now mechanism of fullerene- and nanotube-formation is a controversial point. Many different models have been proposed to explain their formation [41, 56-59, 61, 63-67, 69, 72-92]. The known mechanisms can be categorized into two major groups: bottom-up and top-down models. In the first case, fullerene cages and nanotubes are considered to be formed from carbon atoms and small carbon clusters [41, 56, 57, 59, 64, 69, 72-76, 81, 82, 90–92]. To the first group one could also refer such mechanism as the growth of small endohedral metallofullerenes by 'eating' vaporized carbon [69]. In the second case, fullerenes and nanotubes are thought as direct transformation of graphene into fullerenes or nanotubes [27, 58, 61, 63, 77-79, 83, 85, 86].

There is also a group of researchers interested in cosmic studies [58, 65, 67]. Since a key component of the carbon dust inventory in planetary nebulae are polycyclic aromatic hydrocarbons and their species, the authors suggest various mechanisms of formation five-membered rings in these molecules under irradiation, the molecule dehydrogenation and fusion leading to fullerene formation. One of the recent experimental studies connected with radiation damage is electron-beam-induced transformation of sumanene crystals into carbon cages [89]. Sumanene molecule $C_{21}H_{12}$ with C_{3v} symmetry has three five-membered rings and is considered as a key fullerene fragment together with corannulene $C_{20}H_{10}$ with C_{5v} symmetry having one five-membered ring [93]. From the mechanism viewpoint, these investigations refer to the second group.

Dehydrogenated corannulene was used as a basic structural unit for nucleation of fullerenes and single-walled carbon nanotubes (SWNT) in Ref. [80]. The entities are considered

in the framework of elasticity theory. Existence of curved surfaces introduces forces that depend on the properties of the particular surfaces. The elasticity theory relates the surface tension to the tangential stresses. Any deviation from sphericity deals with stretching as the first-order effect and bending as the second-order one. On the other hand, the conversion of a graphene sheet into cylindrical tubule does not require stretching and bending becomes the first-order effect. Since the nucleation conditions could be different, the cluster of carbon atoms can form the cap of a nanotube or a fullerene. These conclusions received the experimental support in Ref. [86], where at small helium pressure, graphene layers and fullerene-like structures were observed. At high pressure, surface morphology of the anode was changed and evolution of carbon nanotubes was observed.

For completeness sake the studies connected with mathematical description of fullerene and nanotube growth should be mentioned. The typical examples are Refs. [74, 84]. One of them develops the probability-kinetic approach [74], the other uses the theory of diffusion [84]. Both approaches need input parameters that must be obtained from experiments or independent calculations.

Geodesy and topology. Any numerical calculations of fullerene energy and other properties need input data. For small fullerenes the number of possible configurations is not very large, but as one passes to middle-sized fullerenes one obtains a monstrous number of isomers. It is clear that there is no big sense in studying all of them, so it is desirable to restrict their number to the most stable ones. Now there are two restrictive analytical methods [94-98, 100 and references therein, 101]. The first is a combination of graph theory with group theory and could be named geometric modeling. It is based on the principle “the minimum surface at the maximum volume”. It means that a forming fullerene tends to take the form of a perfect spheroid with equal covalent bonds. The geometric modeling allows imagine from the very beginning a possible way of growing carbon clusters and thereby to decrease the number of configurations being worth for studying.

Another new analytical restriction method refers to persistent homology [99]. Homology is formalization of an intuitive idea on confining sets; in this context fullerene set. The authors connected some topological characteristics (barcodes) with the heat of formation and the total curvature energy of fullerene isomers. As any topological method, similar to the graph approach, it needs more precise formulation in order to become a really quantitative method. In the graph approach it was the requirement: symmetry of dimetric representation and graph must be uniform [95-98]. Nevertheless the method of persistent homology is rather interesting since the authors have considered fullerenes and nanotubes in the context of a single theory.

New approach to fullerenes. In Ref. [55] we have enlarged the term “fullerene” upon any convex shape inscribed into a spherical surface which can be composed of atoms, each atom having three nearest neighbors, as in usual fullerenes, whenever discussing hollow carbon clusters. This new approach allowed us to obtain possible forms of mini-fullerenes, from C_4 to C_{20} that, in its turn, allowed filling up a gap between classical fullerenes and small carbon cages including in the list of fullerenes such broad-sense fullerenes. The next step was done in Ref. [95], where the diagrams, showing the formation of mini-fullerenes from single carbon atoms and carbon dimers, were suggested. In addition to the diagrams, here the graph theory was used for analysis of the fullerene structures obtained. The graph analysis allows solving also an inverse problem, i.e. how to predict the ways of producing possible fullerenes, if one knows their graphs [96, 97]. We have designed the structure of some fullerenes from twenty to forty-eight starting at basic mini-fullerenes [91, 97, 98]. It is worth noting that in doing so we have obtained fullerene C_{36} with D_{6h} symmetry. It was synthesized and separated from arc derived carbon soot at UC, Berkeley [18].

Arrhenius’ postulate. In 1889 Svante August Arrhenius postulated that a chemical reaction goes as follows [102] $A + B \leftrightarrow (AB) \rightarrow Y + Z$. It means that at first there forms some

intermediate compound and only afterwards a usual chemical reaction is going on. For fullerenes and nanotubes this postulate leading to fusion reactions can be written in the form $C_n + C_m \rightarrow (C_n C_m) \rightarrow C_{n+m}$. In Ref. [92] 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 which is based on this postulate. Following the postulate we considered recently some fullerene reactions and have obtained fullerenes of the Δn=6 periodicity C_{14}, C_{18}, C_{24}, C_{30} and C_{36} [103]; of Δn=8 periodicity C_{20}, C_{24}, C_{32}, C_{40} and C_{48} [92]; of Δn=10 periodicity C_{26}, C_{30}, C_{40}, C_{50} and C_{60} [104]; of Δn=12 periodicity C_{32}, C_{36}, C_{48}, C_{60} and C_{72} [105]; and of Δn=14 periodicity C_{38}, C_{42}, C_{56}, C_{70} and C_{84} [106].

Aim of study. In radiation solid state physics it is well known that one and the same small vacancy cluster (embryo) during its growth can transform either into a void (volume configuration) or into a dislocation loop (plane configuration) [107]. The question arises whether such situation is possible for elementary fullerenes. Under the elementary fullerenes we understand a tetrahedron, a cube, and triangular, pentagonal and hexagonal prisms which were analyzed carefully in Refs. [55, 95, 96]. Here we think over fullerenes as volume configurations and nanotubes as curved plane configurations. In this contribution we try to answer this question.

2. Reactions of tetrahedral fullerene C_4

Reaction between two tetrahedrons and explanation of some notions. Suppose that two tetrahedral carbon molecules react in the following manner $C_4 + C_4 \rightarrow (C_4 C_4) \rightarrow C_8$. In Figure 1 the atomic configurations corresponding to this reaction are shown. At first two molecules C_4 are moving towards each other (Fig. 1a). Then the atoms, marked with red, interact with each other and produce a compound (Fig. 1b). During this process new covalent bonds (red lines) are formed and old covalent bonds between the reacting atoms (blue dotted lines) are destroyed. As a result, a distorted hexahedron is formed (Fig. 1c) which relaxes into a cube (Fig. 1d).

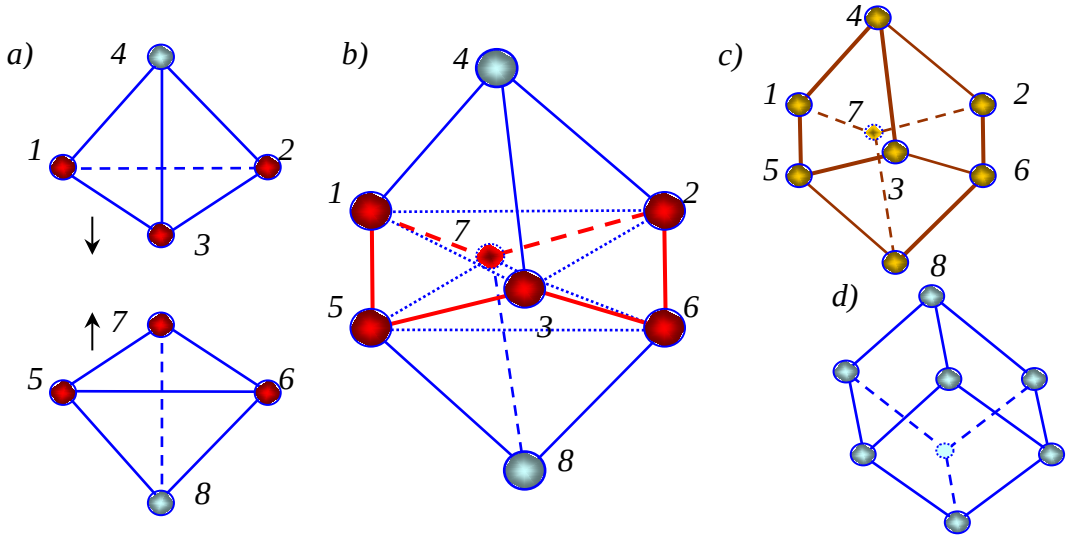

Fig. 1. Joining of two carbon tetrahedrons: *a*) separate tetrahedrons; covalent bonds (blue lines), reacting atoms (red spheres), neutral atoms (blue spheres); *b*) intermediate compound; new covalent bonds (red lines), old covalent bonds to be destroyed (blew dotted lines); *c*) distorted hexagon formed, *d*) hexagon (cube) after relaxation.

One can describe this process with the help of graph theory as it is done in Figure 2. Consider some notions of this theory [108]. Let we have two graphs G_1 and G_2, each graph

having p_i vertices and q_i edges, $i = 1 \vee 2$. If one joins all the vertices of both graphs, one obtains a vertex-connected graph $G_1 + G_2$, where the number of vertices is $p_1 + p_2$, and the number of edges is $q_1 + q_2 + p_1 p_2$. If to remove vertex v_i from graph G_i, one obtains subgraph $G_i - v_i$. In our case we have graph G_1 with vertices 1, 2, 3, 4, and edges 12, 13, 23, 14, 24, 34; and graph G_2 having vertices 5, 6, 7, 8, and edges 56, 57, 67, 58, 68, 78 (Fig. 2a). Since not all the vertices take part in connecting two graphs, we need to exclude non-reactive vertices 4 and 8, as well as edges 14, 24, 34 and 58, 68, 78, connected with these vertices; therefore in reality we need to consider only subgraph $G_1 - v_4$ with vertices 1, 2, 3, and edges 12, 13, 23, and subgraph $G_2 - v_8$.with vertices 5, 6, 7, and edges 56, 57, 67. As a result, one obtains a vertex-connected subgraph $(G_1 - v_4) + (G_2 - v_8)$ with six vertices 1, 2, 3, 5, 6, 7, six old edges 12, 13, 23, 56, 57, 67, and nine new edges 15, 16, 17, 25, 26, 27, 35, 36, 37.

However, applying any mathematical model to physical problems, it is important to keep in mind that except of mathematical rules there are physical restrictions. In our case we must bear in mind that covalent bonds exist only between nearest-neighbor atoms. Therefore we must exclude also edges 16, 25, 37. As a result, we obtain a 'partially' vertex-connected subgraph having six vertices 1, 2, 3, 5, 6, 7, six old edges 12, 13, 23, 56, 57, 67, and six new edges 15, 17, 26, 27, 35, 36 (Fig. 2b). It is clear that analyzing this subgraph is a simpler task.

We supposed that during the reaction of two tetrahedrons new covalent bonds (red lines) are formed and old covalent bonds between the reacting atoms (blue lines) are destroyed. Both types of bonds are shown in the subgraph obtained as edges before destroying (Fig. 2b) and after (Fig. 2c). In the latter the broken bonds (edges) are shown by dotted lines. Here we added the fictitious vertex 7_f in order to show subgraph symmetry. Removing the broken bonds (edges) and adding the non-reactive vertices 4 and 8, as well as their edges 14, 24, 34 and 58, 68, 78, one obtains the graph corresponding to three-fold symmetry of the fullerene formed (Fig. 2d). To avoid the fictitious vertex 7_f, it is reasonable to pass on four-fold symmetry of the fullerene. In doing so one obtains the graph shown in Figure 2e.

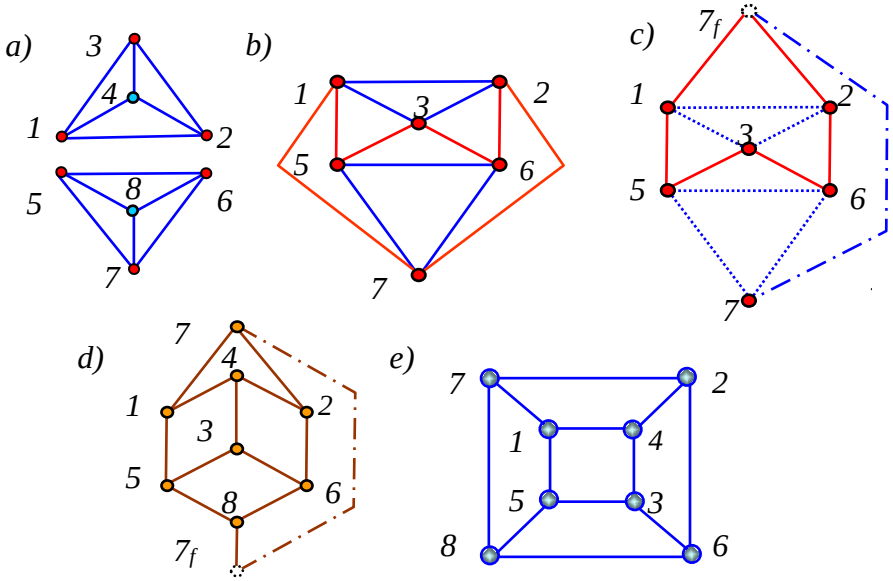

Fig. 2. Graphs: *a*) separate tetrahedrons; edges (blue lines), connectable vertices (red circles), neutral vertices (blue circles), *b*) partial vertex-connected subgraph; new connecting edges (red lines), *c*) removed edges (dotted blue lines), *d*) full graph reflecting three-fold symmetry of fullerene C_8 formed, *e*) full graph reflecting four-fold symmetry of fullerene C_8 formed.

Reactions of tetrahedron C_4 with triangular prism C_6. In Figure 3 the atomic configurations corresponding to reaction $C_4 + C_6 \to (C_4C_6) \to C_{10}$ are shown. At first two molecules are moving towards each other (Fig. 3a). Then the atoms, marked with red, interact with each other to produce a compound (Fig. 3b). During this process new covalent bonds (red lines) are formed and old covalent bonds between the reacting atoms (blue dotted lines) are destroyed. As a result, fullerene C_{10} is formed (Fig. 3c). It is tri-(tetra-penta)$_3$ semiregular septahedron that resembles a lance-head.

Similar to the previous reasoning we can consider this reaction on the basis of graph theory. At first we have two independent graphs (Fig. 4a), then we obtain the partially vertex-connected graph having ten vertices, six stable and six unstable old edges, together with six new formed edges (Fig. 4b), and at last, the graph corresponding to three-fold symmetry of the fullerene formed is composed (Fig. 4c). We see again that analyzing the fullerene reaction in the frame of graph representation is a simpler task. Obviously that it is connected with the fact that the graph approach reduces a three-dimensional problem to a two-dimensional one.

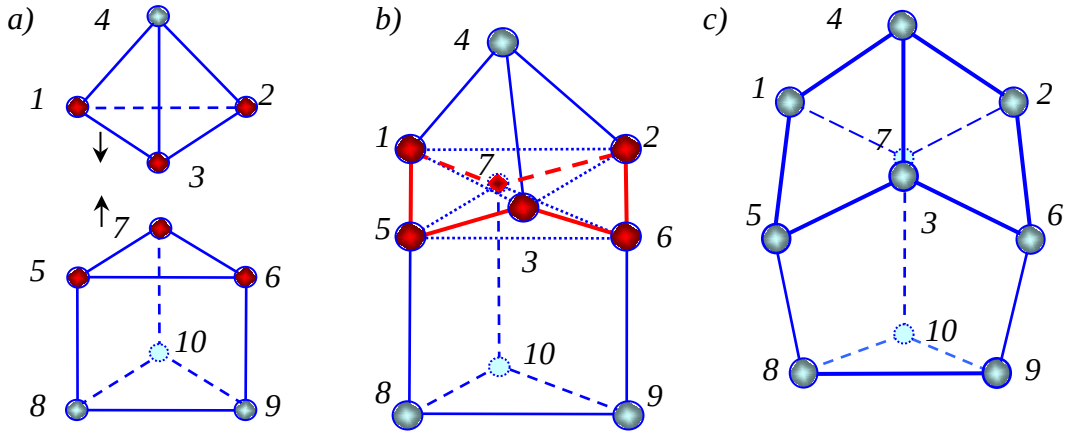

Fig. 3. Joining of a tetrahedron to a triangular-prism: *a*) separate tetrahedron and triangular prim; covalent bonds (blue lines), reacting atoms (red spheres), neutral atoms (blue spheres), *b*) intermediate compound; new covalent bonds (red lines), *c*) semiregular septahedron fullerene C_{10}.

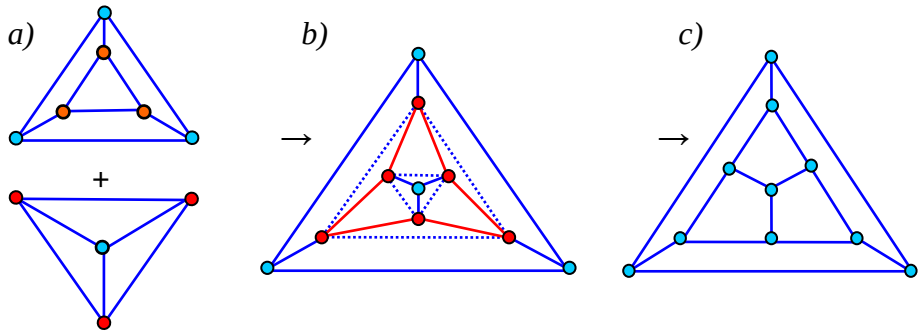

Fig. 4. Connection of graphs: *a*) separate graphs corresponding to a triangular prism (above) and a tetrahedron (below), *b*) connection with physical restrictions, *c*) graph of tri-(tetra-penta)$_3$ fullerene shown in Fig. 3c. All notations are the same as before.

Reaction $C_4 + C_{10} \to (C_4C_{10}) \to C_{14}$**.** Since the graph approach is simpler, we begin with it. At first we have two independent graphs (Fig. 5a), then we obtain the partially vertex-connected graph having fourteen vertices, twelve stable and six unstable old edges, together

with six new formed edges (Fig. 5b), and at last, the final graph is composed (Fig. 5c). This graph corresponds to three-fold symmetry of the fullerene formed (Fig. 5d) and could be named as a tetragonal trefoil-pair (or shamrock-pair) polyhedron. Its energy was calculated in Ref. [103]. In Figure 5e the isomorphic graph of the fullerene is also given. It shows better a structure and symmetry of this polyhedron.

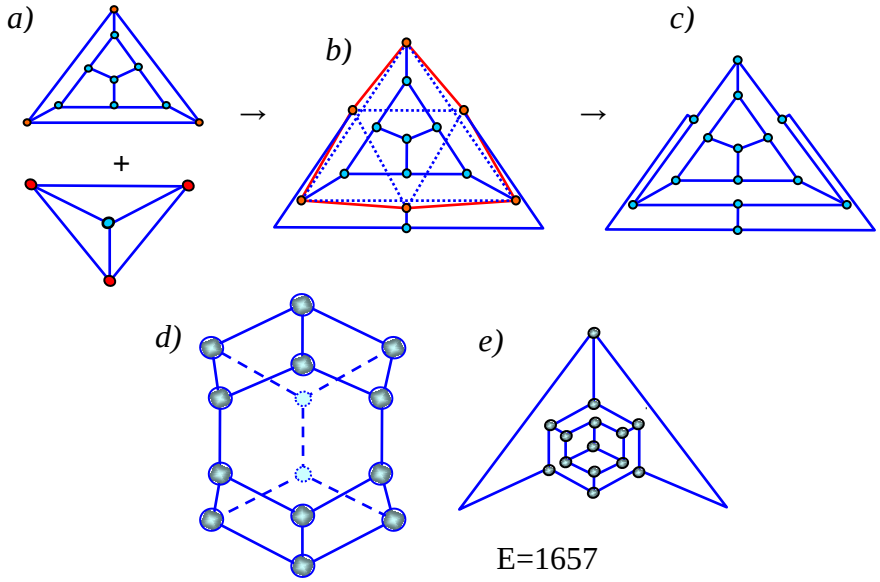

Fig. 5. Connection of graphs: *a*) separate graphs corresponding to a semiregular septahedron fullerene (above) and a tetrahedron (below), *b*) connection with physical restrictions, *c*) final graph, *c*) tetragonal trefoil polyhedron C_{14} obtained, *e*) isomorphic graph. All notations are the same as before.

Reactions of tetrahedron C_4 with triangular barrel C_{12}. This fullerene C_{12} was named in [96] as a triangular barrel-shaped fullerene or a rugby ball. In Ref. [55] possible ways of its formation, initiated both by a reaction-active single atom and by a reaction-active dimer, were considered. The ways resemble formation of a zigzag polymer during polymerization. In Ref. [96] it was suggested that the fullerene can be also originated from a three-atom cluster. Reaction $C_4 + C_{12} \rightarrow (C_4C_{12}) \rightarrow C_{16}$ is displayed in Figure 6 as a connection of graphs, together with a fullerene obtained.

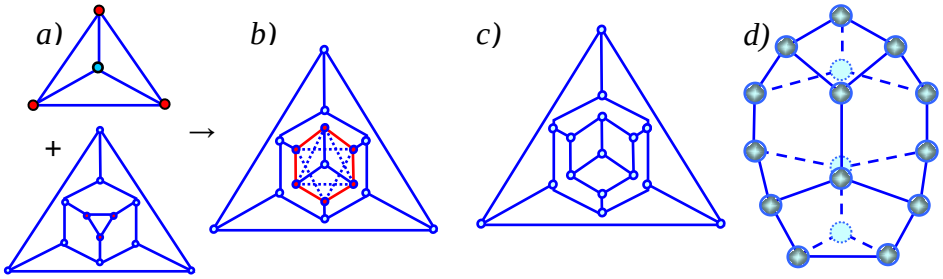

Fig. 6. Connection of graphs: *a*) separate graphs corresponding to a tetrahedron (above) and a triangular barrel-shape polyhedron (below), *b*) connection with physical restrictions, *c*) final graph of semiregular decahedron C_{14} (*d*). All notations are the same as before.

Reaction $C_4 + C_{16} \rightarrow (C_4C_{16}) \rightarrow C_{20}$ is shown in Figure 7 as a connection of graphs, together with a fullerene obtained. Contrary to the semiregular decahedron that can be inscribed in an ellipsoid and therefore can be identified as a fullerene, the irregular dodecahedron resembles more a two-closed-end mini-nanotube.

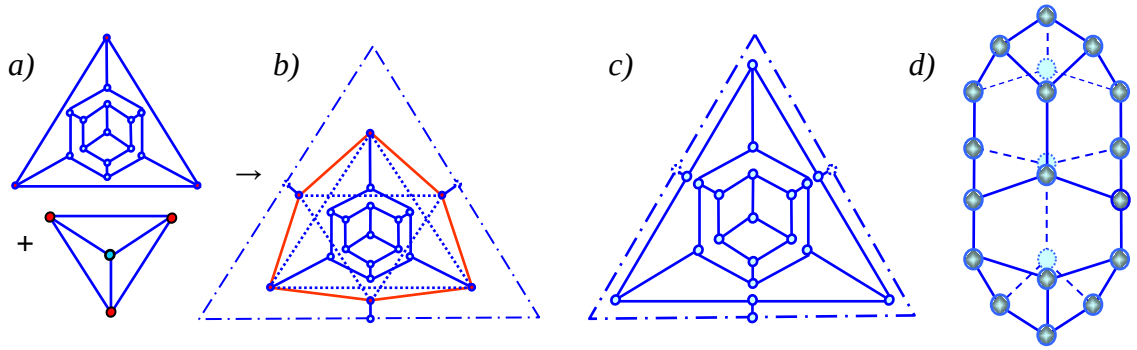

Fig. 7. Connection of graphs: *a*) separate graphs corresponding to a semiregular decahedron (above) and a tetrahedron (below), *b*) connection with physical restrictions, *c*) final graph of an irregular dodecahedron (d). All notations are the same as before.

3. Reactions of triangular-prism fullerene C_6

Reaction between two triangular prisms can be written as $C_6 + C_6 \rightarrow (C_6C_6) \rightarrow C_{12}$ and is presented in Figure 8 as a connection of graphs, together with a fullerene obtained. As already noted the fullerene was named in [2, 3] as a triangular barrel-shaped fullerene or a rugby ball. In [2] a possible way of its formation, initiated by a reaction-active single atom as well as by a reaction-active dimer, was considered. The way resembles formation of a zigzag polymer during polymerization. In [3] it was suggested that the fullerene can be also originated from a three-atom cluster. Now we have the third way of this fullerene formation.

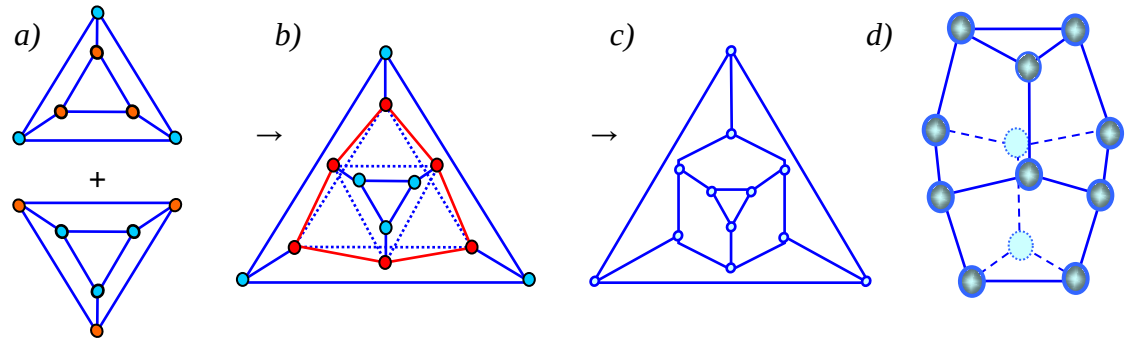

Fig. 8. Connection of graphs: *a*) separate graphs corresponding to triangular prisms; *b*) connection with physical restrictions; *c*) final graph of a triangular barrel-shaped fullerene (d). All notations are the same as before.

Reaction of triangular prism C_6 and barrel C_{12} $C_6 + C_{12} \rightarrow (C_6C_{12}) \rightarrow C_{18}$ is exhibited in Figure 9 as connection of graphs, together with a fullerene obtained. The fullerene was named in Refs. [2, 3] as a truncated bi-shamrock. Some possible ways of forming this cluster initiated by a reaction-active single atom as well as by a reaction-active dimer, were suggested in [2]. Now they seem us too complex in comparison with that of considered here.

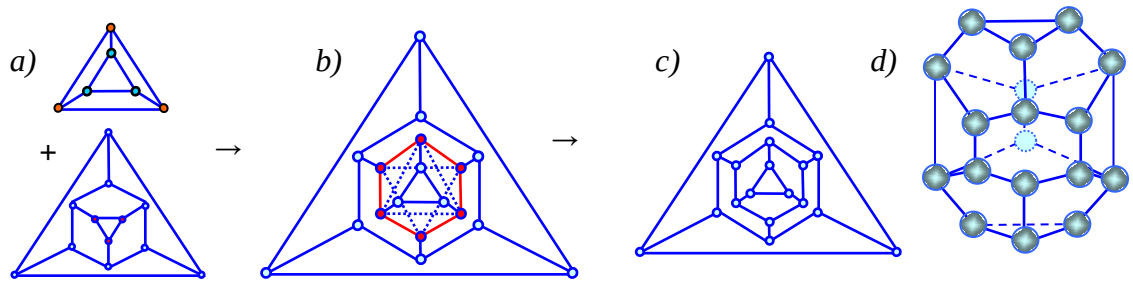

Fig. 9. Connection of graphs: *a*) separate graphs corresponding to a triangular prism (above) and a triangular barrel-shaped fullerene (below), *b*) connection that takes into account physical restrictions, *c*) final graph of truncated bi-shamrock fullerene C_{18} (d). All notations are the same as before.

Reaction $C_6 + C_{16} \to (C_6C_{16}) \to C_{22}$ is illustrated in Figure 10 as connection of graphs, together with a cluster obtained. The carbon cluster is a one closed-end mini-nanotube. Contrary to the irregular dodecahedron with closed ends (Fig. 7d), this nanotube is able to growing by adding triangular prisms as it shown in Figure 10e. The corresponding reactions can be written as follows

$C_6 + C_{22} \to C_{28}$, $C_6 + C_{28} \to C_{34}$, … $C_6 + C_N \to C_{N+6}$. $N = 16 + 6n$, $n = 1, 2, \ldots$.

It is clear that the growth of the nanotube will be stopped if instead of adding triangular prisms, tetrahedrons are appended to the nanotube. In this case one obtains nanotubes according to the reactions

$C_4 + C_{16} \to C_{20}$, $C_4 + C_{22} \to C_{26}$, $C_4 + C_{28} \to C_{32}$, … $C_4 + C_N \to C_{N+4}$. $N = 16 + 6n$, $n = 1, 2, \ldots$

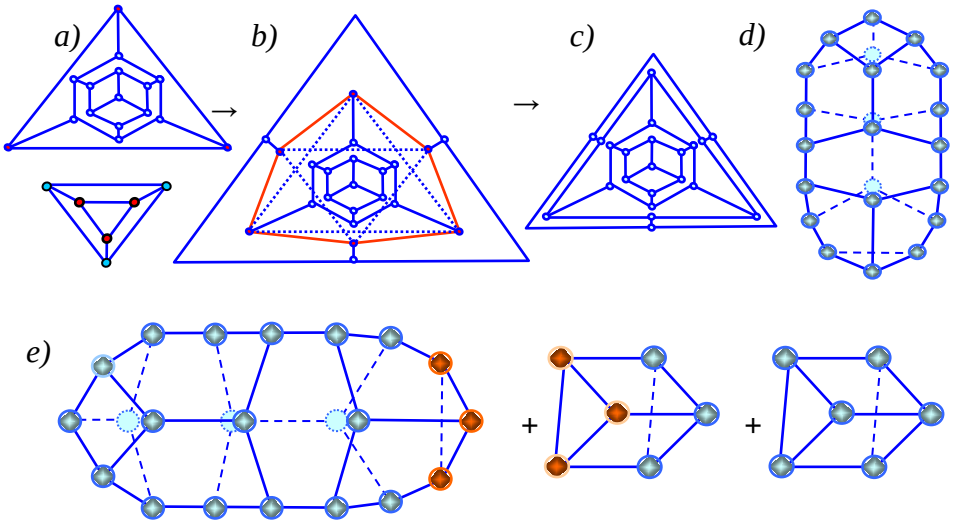

Fig. 10. Connection of graphs: *a*) separate graphs corresponding to an irregular decahedron (above) and a triangular prism (below), *b*) connection with physical restrictions, *c*) final graph of a nanotube (*d*); *e*) growth of the nanotube obtained.

Reaction $C_6 + C_{18} \to (C_6C_{18}) \to C_{24}$ is presented in Figure 11 as connection of graphs, together with a cluster obtained. The carbon cluster is an opened-end mini-nanotube. Contrary to the previous case, this nanotube is able to growing by adding triangular prisms to both ends. The corresponding reactions can be written as follows

$C_6 + C_{24} \to C_{30}$, $C_6 + C_{30} \to C_{36}$, … $C_6 + C_N \to C_{N+6}$. $N = 18 + 6n$, $n = 1, 2, \ldots$

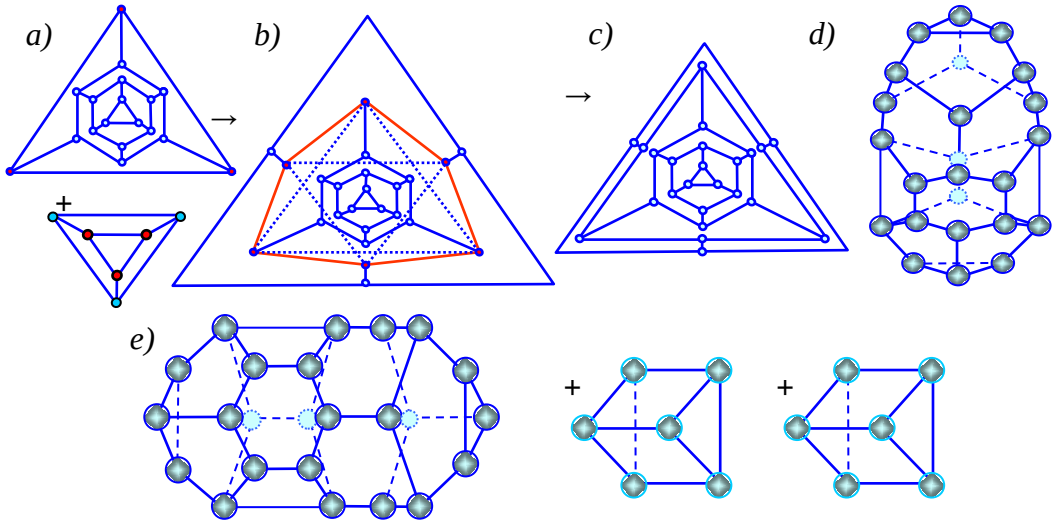

Fig. 11. Connection of graphs: *a*) separate graphs corresponding to a bi-shamrock (above) and a triangular prism (below), *b*) connection with physical restrictions, *c*) final graph of a nanotube (*d*); *e*) growth of the nanotube obtained.

4. Reactions of cube fullerene C_8

Reaction between two cubes can be written as $C_8 + C_8 \to (C_8C_8) \to C_{16}$. Its graph representation is shown in Figure 12a. One of two initial cubes and a final geometric body are illustrated in Figure 12b.

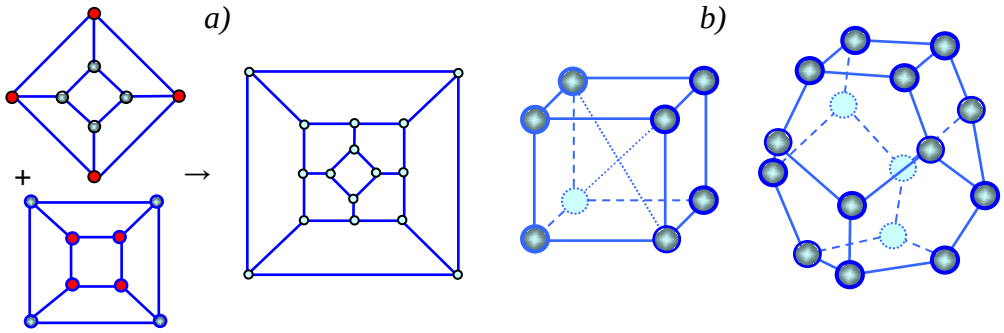

Fig. 12. Fusion of two cubes as connection of their graphs (*a*); *b*) cube and square barrel-shape fullerene C_{16}.

Reactions of cube C_8 with square barrel C_{16} $C_8 + C_{16} \to (C_8C_{16}) \to C_{24}$ is presented in Figure 13 as connection of graphs, together with a fullerene formed. The final graph was designed earlier in Ref. [4] on different geometrical grounds, but the fullerene structure was not given. One can consider this carbon cluster not only as a fullerene, but an opened-end mini-nanotube as well. This nanotube is able to growing by adding carbon cubes to both ends. The corresponding reactions are

$C_8 + C_{24} \to C_{32}$, $C_8 + C_{32} \to C_{40}$, … $C_8 + C_N \to C_{N+6}$. $N = 16 + 8n$, $n = 1, 2, \ldots$

It is worth noting that similar nanotube with n=8, N=80 was studied in Ref. [76].

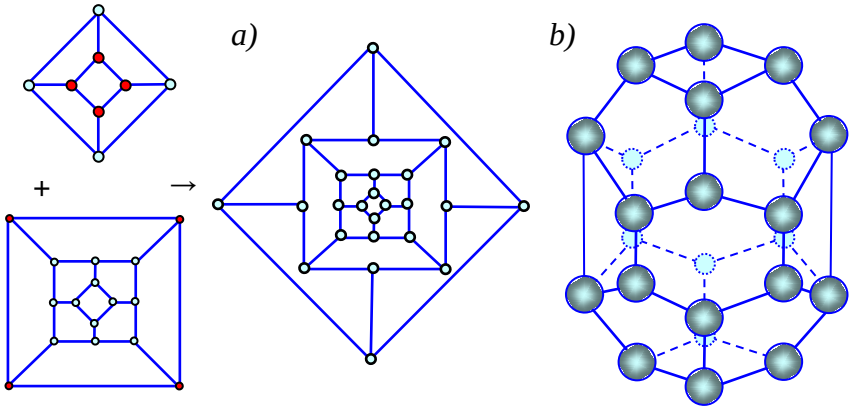

Fig. 13. Connection of graphs: *a*) separate graphs of a cube (above) and a square barrel-shape fullerene (below), as well as their connection; *b*) fullerene C_{24} obtained.

5. Reactions of pentagonal prism C_{10}

Reaction between two pentagonal prisms is written as $C_{10} + C_{10} \to (C_{10}C_{10}) \to C_{20}$. It is shown both as a graph connection and as an initial and a final geometric body in Figure 14.

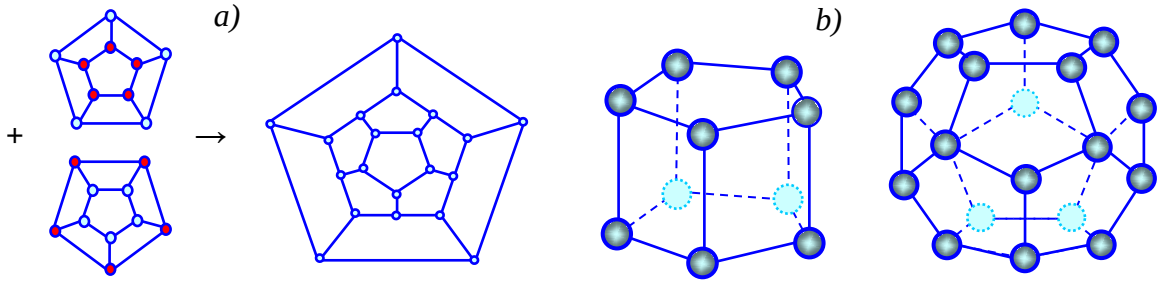

Fig. 14. Fusion of two pentagonal prisms as connection of their graphs (*a*); *b*) pentagonal prism and five-cornered barrel-shape fullerene (dodecahedron).

Reactions of prism C_{10} with dodecahedron C_{20} $C_{10} + C_{20} \to (C_{10}C_{20}) \to C_{30}$ is exhibited in Figure 15 as connection of graphs, together with a fullerene formed. The final graph was designed earlier [4] on different geometrical grounds, but the fullerene structure was not given. Similar to the previous case, this carbon cluster is not only a fullerene, but an opened-end mini-nanotube as well. This nanotube is able to growing by adding carbon pentagonal prisms to both ends. The corresponding reactions can be written as follows

$C_{10} + C_{30} \to C_{40}$, $C_{10} + C_{40} \to C_{50}$, … $C_{10} + C_N \to C_{N+10}$. $N = 20 + 10n$, $n = 1, 2, \ldots$

It is worth noting that such nanotube with n=6, N=80 was also studied in [76].

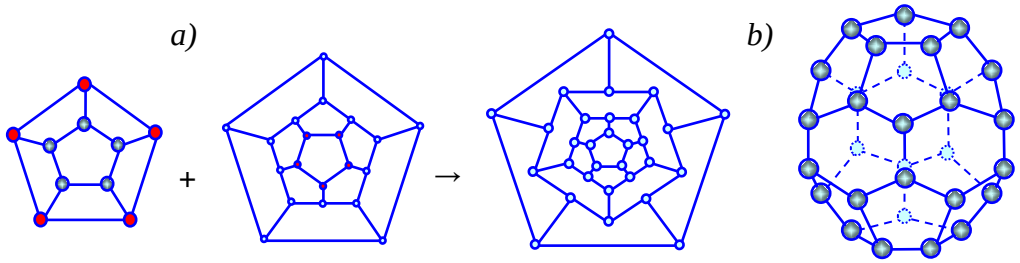

Fig. 15. Connection of graphs: *a*) separate graphs of a pentagonal prism and a five-cornered barrel-shape fullerene, as well as their connection; *b*) fullerene C_{30} obtained.

6. Reactions of hexagonal prism C_{12}

Reaction between two hexagonal prisms is written as $C_{12} + C_{12} \to (C_{12}C_{12}) \to C_{24}$ and is shown both as a graph connection and as an initial and a final geometric body in Figure 16.

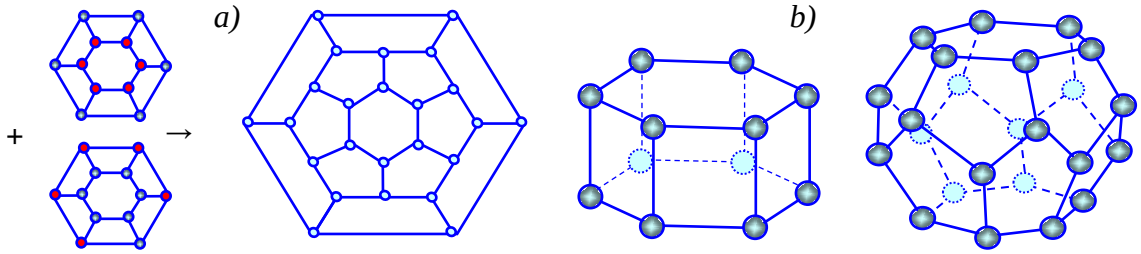

Fig. 16. Fusion of two hexagonal prisms as connection of their graphs (*a*); *b*) hexagonal prism and six-cornered barrel-shape fullerene C_{24}.

Reactions of prism C_{12} with barrel fullerene C_{24} $C_{12} + C_{24} \to (C_{12}C_{24}) \to C_{36}$ is presented in Figure 17 as connection of graphs, together with a fullerene formed. The final graph was designed earlier [4] on different geometrical grounds, but the fullerene structure was not given. Similar to the previous case one can consider this carbon cluster not only as a fullerene, but an opened-end mini-nanotube as well. This nanotube is able to growing by adding carbon cubes to both ends. The corresponding reactions are as follows

$C_{12} + C_{36} \to C_{48}$, $C_{12} + C_{48} \to C_{60}$, … $C_{12} + C_N \to C_{N+12}$. $N = 24 + 12n$, $n = 1, 2, \ldots$

It is worth noting that such nanotube with n=6, N=96 was also studied in [76].

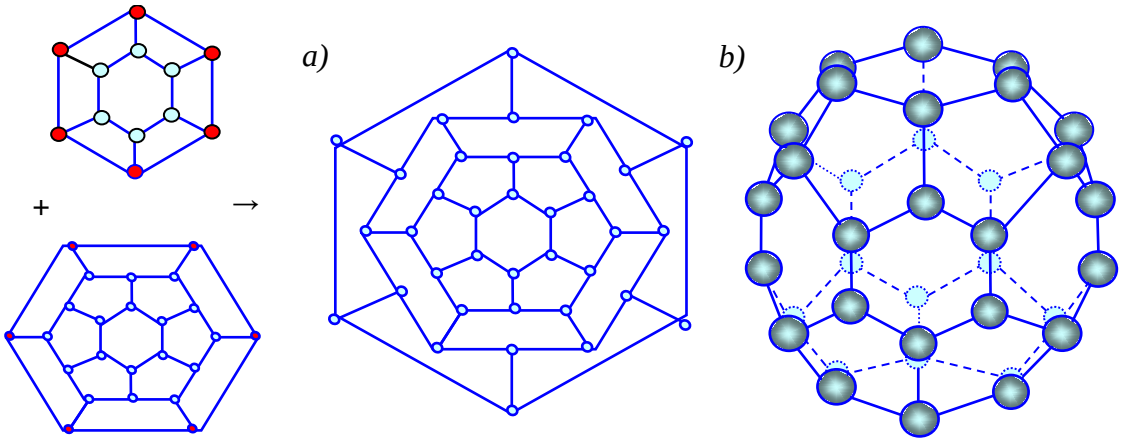

Fig. 17. Connection of graphs: *a*) separate graphs corresponding to a hexagonal prism (above) and a six-cornered barrel-shape fullerene (below), as well as their connection with physical restrictions; *b*) fullerene C_{36} obtained.

7. Conclusion

We have considered reactions of elementary fullerenes (from C_4 to C_{12}) with each other as well as with their heirs. Under the elementary fullerenes we understand a tetrahedron, a cube, and triangular, pentagonal and hexagonal prisms. The process is similar to fusion of bubbles in a soap solution. The graphs describing the process are suggested. The reaction zone is a vertex-connected subgraph that takes into account physical restrictions, namely that covalent bonds exist only between nearest-neighbor atoms. We supposed that during the reactions new covalent bonds are formed and old covalent bonds between the reacting atoms are destroyed. In doing

so we obtained the carbon clusters that refer to fullerenes and nanotubes. It was found that elementary fullerenes can transform either into larger fullerenes or into nanotubes reacting with similar fullerenes of the same symmetry and their successors.

References

[1] H.W. Kroto, J.R. Hearth, S.C. O'Brien, R.F. Curl, R.E. Smalley, C60: Buckminsterfullerene // *Nature* **318** (1985) 162.
[2] H.W. Kroto, The stability of the fullerenes Cn, with n=24, 28, 32, 36, 60, 60 and 70 // *Nature* **329** (1987) 529.
[3] S. Iijima, Helical microtubules of graphitic carbon // *Nature* **354** (1991) 56.
[4] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Electrical field effect in atomically thin carbon films // *Science* **306** (2004) 666.
[5] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos, A.A. Firsov, Two-dimensional gas of massless Dirac fermions in graphene // *Nature* **438** (2005) 197.
[6] *Nanostructured Carbon for Advanced Applications*, edited by G. Benedek, P. Milani and V.G. Ralchenko (Kluwer Academic Publishers, Dordrecht, 2001) NATO Science Series II. Mathematics, Physics and Chemistry. Vol. 24.
[7] *Perspectives of Fullerene Nanotechnology*, edited by Eiji Ōsawa (Kluwer Academic Publishers, Dordrecht, 2002).
[8] *Carbon Nanotubes*, edited by Valentin N. Popov and Philippe Lambin (Springer, Dordrecht, 2006) NATO Science Series II. Mathematics, Physics and Chemistry. Vol. 222.
[9] *Contemporary Concepts of Condensed Matter Science*, Series Editors E. Burstein, M.L. Cohen, D.L. Mills and P.J. Stiles. *Carbon Nanotubes: Quantum Cylinders of Graphene*, Volume Editors S. Saito and A. Zettle (Elsevier, Amsterdam, 2008).
[10] *Handbook of Nanophysics. Clusters and Fullerenes*, edited by Klaus D. Sattler (CRC Press, Taylor and Francis Group, LLC, 2010).
[11] *Graphene. Synthesis and Applications*, edited by Wongbong Choi and Jo-won Lee (CRC Press, Taylor and Francis Group, LLC, 2012).
[12] B.S. Murty, P. Shankar, Badlev Raj, B.B. Rath, James Murday, *Textbook of Nanoscience and Nanotechnology* (Springer University Press, India, 2013).
[13] *Springer Handbook of Nanomaterials*, edited by Robert Vajtai (Springer-Verlag, Berlin, 2013).
[14] *Carbon Nanomaterials*, Second Edition, edited by Yuri Gogotsi and Volker Presser (CRC Press, Taylor and Francis Group, LLC, 2014).
[15] Debaprasad Das, Hafizu Rahaman, *Carbon Nanotubes and Graphene Nanoribbon Interconnects* (CRC Press, Taylor and Francis Group, LLC, 2015).
[16] *Carbon Nanomaterials Sourcebook*, Vol. 1. *Graphene, Fullerenes, Nanotubes, and Nanodiamonds*, edited by Klaus D. Sattler (CRC Press, Taylor and Francis Group, LLC, 2016).
[17] *Structure and Multiscale Mechanics of Carbon Nanomaterials*, edited by Oscar Paris, CISM International Centre for Mechanical Sciences 563 (Springer, Wien, CISM, Udine, 2016).
[18] C. Piskoti, J. Yarger, A. Zettl, C36, a new carbon solid // *Nature* **393** (1998) 771.
[19] H. Prinzbach, A. Weiler, P. Landenberger, F. Wahl, J. Wörth, L.T. Scott, M. Gelmont, D. Olevano, B.V. Issendorf, Gas-phase production and photoelectron spectroscopy of the smallest fullerene C20 // *Nature* **407** (2000).
[20] D.E. Manolopoulos, J.C. May, and S.E. Down, Theoretical studies of the fullerenes: C34 to C70 // *Chem. Phys. Lett*. **181** (1991) 105.

[21] T. Guo, M.D. Diener, Y. Chai, A.J. Alford, R.E. Haufler, S.M. McClure, T. Ohno, J.H. Weaver, G.E. Scuseria, R.E. Smalley, Uranium stabilization of C28 – a tetravalent fullerene // *Science* **257** (1992) 1661.
[22] B.L. Zhang, C.Z. Wang, K.M. Ho, C.H. Xu, and C.T. Chan, The geometry of small fullerene cages: C20 to C70 // *J. Chem. Phys*. **97** (1992) 5007.
[23] B.L. Zhang, C.H. Xu, C.Z. Wang, C.T. Chan, and K.M. Ho, Systematic study of structures and stabilities of fullerenes // *Phys. Rev*. B **46** (1992) 11.
[24] J.C. Grossman, M. Cote, S.G. Louie, M.L. Cohen, Electronic and structural properties of molecular C36 // *Chem. Phys. Lett*. **284** (1998) 344.
[25] M.N. Jagadeesh, J. Chandrasekhar, Computational studies on C36 and its dimer // *Chem. Phys. Lett.* **305** (1999) 298.
[26] A. Ito, T. Monobe, T. Yoshii, K. Tanaka, Electronic structures of C36 fulleride anions: $C36^{-}$ and $C362^{-}$ // *Chem. Phys. Lett*. **315** (1999) 348.
[27] A.I. Melker, S.N. Romanov, D.A. Kornilov, Computer simulation of formation of carbon fullerenes // *Materials Phys. Mech*. **2** (2000) 42.
[28] N. Breda, R.A.Broglia, G. Colo, G. Onida, D. Provasi, E. Vigezzi, C28: a possible room temperature organic superconductor // *Phys. Rev*. B **62** (2000) 130.
[29] Z. Chen, H. Jiao, M. Bühl, A. Hirsch, W. Thiel, Theoretical investigation into structures and magnetic properties of smaller fullerenes and their heteroanalogues // *Theor. Chem. Acc.* **106** (2001) 352.
[30] D.A. Kornilov, A.I. Melker, S.N. Romanov, New molecular dynamics predicts fullerene formation // *Proc. SPIE* **4348** (2001) 146.
[31] B. Paulus, Electronic and structural properties of the cage-like molecules C20 to C36 // *Phys. Chem. Chem. Phys*. **5** (2003) 3364.
[32] Z.X. Zhang, Z.Y. Pan, Y.X. Li, Q. Wei, Simulations of the nanomechanical properties of compressed small fullerenes // *Modern Phys. Lett*. B. **17** (2003) 877.
[33] S.Y. Xie, F. Gao, X. Lu, R.B. Huang, C.R. Wang, X. Zhang, M.L. Liu, S.L. Deng, L.S. Zheng, Capturing the labile fullerene C_{50} as $C_{50}Cl_{10}$ // *Science* **304** (2004) 699.
[34] A.I. Melker, Fullerenes and nanotubes: molecular dynamics study // *Proc. SPIE* **5400** (2004) 54.
[35] J. Pattanayak, T. Kar, S. Scheiner, Substitution patterns in mono BN-fullerenes: Cn (n = 20, 24, 28, 32, 36 and 40) // *J. Phys. Chem*. A **108** (2004) 7681.
[36] G. Sun, M.C. Nicklaus, R. Xie, Structure, stability, and NMR properties of lower fullerenes C38-C50 and azafullerene C44N6 // *J. Phys. Chem*. A **109** (2005) 4617.
[37] X. Lu, Z. Chen, Curved pi-conjugation, aromaticity, and the related chemistry of small fullerenes (<C60) and single-walled carbon nanotubes // *Chem. Rev*. **105** (2005) 3643.
[38] J. Song, M. Vaziri, A study on electronic and structural properties of C28 and C16N12 // *Mol. Phys*. **104** (2006) 319.
[40] H.S. Kang, A theoretical study of fullerene–ferrocene hybrids // *J. Phys. Chem*. A **110** (2006) 4780.
[41] S.D. Khan, S. Ahmad, Modelling of C2 addition rout to the formation of C60 // *Nanotechnology* **17** (2006) 18.
[42] A.I. Melker, Fifth anniversary of molecular dynamics // *Proc. SPAS jointly with UWM* **10** (2006) 56.
[43] E. Malolepsza, H.A. Witek, S. Irle, Comparison of geometric, electronic, and vibrational fullerenes C20–C36 // *J. Phys. Chem*. A **111** (2007) 6649.
[44] N. Shao, Y. Gao, X.C. Zeng, Search for lowest-energy fullerenes 2: C38 to C80 and C112 to C120 // *J. Phys. Chem*. C **111** (2007) 17671.
[45] A.I. Melker, Fifth anniversary of molecular dynamics // *Proc. SPIE* **6597** (2007) 659702-1.

[46] A.J.C. Varandas, An ab initial study of the interaction between He and C36 with extrapolation to the one electron basis set limit // *Chem. Phys. Lett.* **463** (2008) 225.
[47] L. Shi, B. Chen, J. Zhou, T. Zhang, Q. Kang, M. Chen, Structure and relative stability of drum-like C4nN2n (n = 3-8) cages and their hydrogenated product C4nH4nN2n (n = 3-8) cage // *Phys. Chem*. A **112** (2008) 11724.
[48] E. Malolepsza, Y. Lee, H.A. Witek, S. Irle, C. Lin, H. Hsieh, Comparison of geometric, electronic, and vibrational properties for all pentagon/hexagon-bearing isomers of fullerenes C38, C40, and C42 // *Int. J. Quantum Chem*. **109** (2009) 1999.
[49] L.-H. Gan, J. Liu, Q. Hui, S.-Q. Shao, Z.-H. Liu, General geometrical rule for stability of carbon polyhedral // *Chem. Phys. Lett.* **472** (2009) 224.
[50] Y-M. Chen, J. Shi, L. Rui, Q-X. Guo, Theoretical study on C32 fullerenes and their endohedral complexes with noble gas atoms // *J. Mol. Struct. THEOCHEM* **907** (2009) 104.
[51] D. Holec, M.A. Hartmann, F.D. Fischer, F.G. Rammerstorfer, P.H. Mayrhofer, O. Paris, Curvature-induced excess surface energy of fullerenes: density functional theory and Monte Carlo simulations // *Phys. Rev*. B **81** (2010) 235403.
[52] F. Lin, E.S. Sørensen, C. Kallin. A.J. Berlinsky, C20, the smallest fullerene. In: *Handbook of Nanophysics. Clusters and Fullerenes*, edited by Klaus D. Sattler, (CRC Press, Taylor and Francis Group, LLC, 2010) p. 29-1.
[53] J. An, L.-H. Gan, J.-Q. Zhao, A global search for the lowest energy isomer of C26 // *J. Chem. Phys* **132** (2010) 154304.
[54] F. Naderi, S. Rostamian, B. Naderi, A study on the electronic and structural properties of fullerene C36 and its interaction with amino acid // *Int. J. Phys. Sci*. **7** (2012) 2006.
[55] A.I. Melker, V. Lonch, Atomic and electronic structure of mini-fullerenes: from four to twenty // *Materials Phys. Mech*. **13** (2012) 22.
[56] P.W. Dunk, N.K. Kaiser, C.L. Hendrickson, J.P. Quin, S.P. Ewels, Y. Nakanischi, S. Sasaki, H. Shinohara, A.G. Marshall, H.W. Kroto, Bottom-up formation of endohedral monometallofullerenes // *Nature Comm*. **352** (2012) 139.
[57] P.W. Dunk, N.K. Kaiser, M. Mulet-Gas, A. Rodríguez-Fortea, J.M. Poblet, H. Shinohara, C.L. Hendrickson, A.G. Marshall, H.W. Kroto, The smallest stable fullerene, M@C28 (M=Ti, Zr, U): stabilization and growth from carbon vapor // *J. Am. Chem. Soc*. **134** (2012) 9380.
[58] E.L. Micelotta, A.P. Jones, J. Cami, E. Peeters, The formation of cosmic fullerenes from arophatic clusters // *Astrophys. J*. **761** (2012) 35.
[59] S-L. Deng, S-Y. Xie, R-B. Huang, L-S. Zheng, The formation mechanism of fullerene // *Sci. Sinica Chim*. **42** (2012) 1587.
[60] A. Kharlamov, G. Kharlamova, M. Bondarenko, V. Fomenko, Joint synthesis of small carbon molecules (C3-C11), quasi-fullerenes (C40, C48, C52) and their hydrides // *Chem. Engng. Sci.* **1** (2013) 32.
[61] J. Zhang, F.L. Bowels, D.W. Bearden, W.K. Ray, T. Fuhrer, Y. Ye, C. Dixon, K. Harich, R.F. Helm, M.M. Olmstead, A.L. Balch, H.C. Dorn, A missing link in the transformation from asymmetric to symmetric metallofullerene cages implies a top-down fullerene formation mechanism // *Nature Chem*. **5** (2013) 880.
[62] F. Naderi, A computational study on the smallest exohedrally functionalized fullerenes, C20X8 (X=H, F, Cl, Br, NH2, OH and CN) // *Bulgarian Chem. Comm*. **4** (2014) 680.
[63] F. Pietrucci, W. Andreoni, Fate of a graphene flake; a new rout toward fullerenes disclosed with ab initio simulations // *J. Chem. Theory Comput*. **10** (2014) 913.
[64] P.W. Dunk, M. Mulet-Gas, Y. Nakanishi, N.K. Kaiser, A. Rodrigues-Fortea, H. Shinohara, J.P. Poblet, A.G. Marshall, H.W. Kroto, Botom-up formation of endohedral metallofullerenes is directed by charge transfer // *Nature Comm*. **5** (2014) 5844.

[65] J. Zhen, P. Castellanos, D.M. Paardekooper, Laboratory formation of fullerenes from PAHs: top-down interstellar chemistry // *Astrophys. J. Lett.* **797** (2014) L30.
[66] R. Sure, R. Tonner, P. Schwerdtfeger, A systematic study of rare gas atoms encapsulated in small fullerenes using dispersion corrected density functional theory // *J. Comp. Chem*. **36** (2015) 88.
[67] P.W. Dunk, H. Niwa, H. Shinohara, A.G. Marshall, H.W. Kroto, Large fullerenes in mass spectra // *Mol. Phys*. **113** (2015) 2359.
[68] Y. Jin, A. Perera, V.F. Lotrich, R.J. Bartlett, Couple cluster geometries and energies of C20 carbon cluster isomers // *Chem. Phys. Lett*. **629** (2015) 76.
[69] M. Mulet-Gas, L. Abella, P.W. Dunk, A. Rodrigues-Fortea, H.W. Kroto, J.P. Poblet, Small endohedral metallofullerenes: exploration of the structure and growth mechanism in $Ti@C_{2n}$ (n=26-50) family // *Chem. Sci*. **6** (2015) 675.
[70] S.D. Bolboacă, L. Jäntschi, Nanoquantitative structure-property relationship modeling on C_{42} fullerene isomers // *J. Chem*. **2016** (2016) ID 1791756.
[71] H.W. Kroto, The stability of the fullerenes C_n, with n = 24, 28, 32, 36, 50, 60 and 70 // *Nature* **329** (1987) 529.
[72] M. Endo, H.W. Kroto, Formation of carbon nanofibers // *J. Phys. Chem*. **96** (1992) 6941.
[73] R. Kerner, Nucleation and growth of fullerenes // *Comp. Mater. Sci*. **2** (1994) 500.
[74] R. Kerner, R.H. Bennemann, Theory for the growth of fullerenes // *Fullerene Sci. Tech*. **4** (1996) 1279.
[75] N.S. Goroff, Mechanism of fullerene formation // *Acc. Chem. Res*. **29** (1996) 77.
[76] Z. Slanina, X. Zhao, F. Uhlik, Model narrow nanotubes related to C36, C32 and C20: initial computational structural sampling // *Mater. Sci. Engng* B **96** (2002) 164.
[77] A.I. Melker, D.A. Kornilov, S.N. Romanov, N.A. Izotova, Carbon nanotubes: formation and computer simulations // *Proc. SPIE* **5127** (2003) 76.
[78] D.A. Kornilov, A.I. Melker, S.N. Romanov, Conformation transitions in fullerenes at non-zero temperatures // *Proc. SPIE* **5127** (2003) 81.
[79] A.I. Melker, Fullerenes and nanotubes. Molecular dynamics study // *Proc. SPIE* **5400** (2004) 54.
[80] S. Ahmad, Criteria for the growth of fullerenes and single-walled carbon nanotubes in sooting environments // *Nanotech*. **16** (2005) 1739.
[81] G. Brinkmann, D. Franceus, P.W. Fowler, J. Graver, Growing fullerenes from seed: growth transformations of fullerene polyhedral // *Chem. Phys. Lett*. **428** (2006) 386.
[82] Y. Yamaguchi, L. Colombo, Growth of $sp\text{-}sp^2$ nanostructures in a carbon plasma // *Phys. Rev*. B. **76** (2007) 134119.
[83] A.I. Melker, Fiftieth anniversary of molecular dynamics // *Proc. SPIE* **6597** (2007) 02.
[84] J.E. Bunder, J.M. Hill, Diffusive growth of fullerenes and carbon nanotubes // *J. Chem. Phys.* **131** (2009) 244703.
[85] A. Chuvilin, U. Kaiser, E. Bichoutskaia, N.A. Besley, A.N. Khlobystov. Direct transformation of grapheme to fullerene // *Nature Chem*. **2** (2010) 450.
[86] V. Gupta, Graphene as intermediate phase in fullerene and carbon nanotube growth: a Young-Laplace surface-tension model // *Appl. Phys. Lett*. **97** (2010) 181910.
[87] S. Irle, A. J. Page, B. Saha, Y. Wang, K.R.S. Chandrakumar, Y. Nishimoto, H-J. Qian, K. Morokuma, Atomistic mechanisms of carbon nanostructure self-assembly as predicted by nonequilibrium QM/MD simulations. In: *Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends,* eds. J. Leszczynski and M.K. Shukla (Springer-European Academy of Sciences, 2012).
[88] P.W. Dunk, N.K. Kaiser, C.L. Hendrickson, J.P. Quinn, C.P. Eweis, Y Nakanishi, H. Shinohara, A.G. Marshall, H.W. Kroto, Closed network growth of fullerenes // *Nature Com.* **3** (2012). doi: 10.1038/ncomms1853.

[89] J. Fujita, M. Tachi, K. Murakami, H. Sakurai, Y. Morita, S. Higashibayashi, M. Takeguchi, Beam-induced graphitic carbon cage transformation from sumanene aggregates // *Appl. Phys. Lett.* **104** (2014) 043107.
[90] N.A. Poklonski, S.V. Ratkevich, S.A. Vyrko, Quantum-chemical calculation of carbododecahedron formation in carbon plasma // *J. Phys. Chem*. A **119** (2015) 9133.
[91] A.I. Melker, M.A. Krupina, Geometric modeling of midi-fullerenes growth from C_{24} to C_{48} // *St. Petersburg State Polytechnical University Journal. Physics and Mathematics* **3(248)** (2016) 52.
[92] A.I. Melker, T.V. Vorobyeva, Fusion reactions of cupola half-fullerenes // *St. Petersburg State Polytechnical University Journal. Physics and Mathematics* **3(248)** (2016) 59.
[93] T. Hiraro, H. Sakurai, First and practical synthesis of sumanene, a C_{3v} symmetric partial structure of fullerene // *Ann. Report Osaka Univ*. **5** (2004) 27.
[94] J.E. Graver, Y.A. Monachino, Highly symmetric fullerenes and nanotubes. In: *Symmetry: Culture and Science. Special issue: Symmetry in Nanostructure*, edited by Mircea Duidea (2008) Vol. 19, pp.317-340.
[95] A.I. Melker, Possible ways of forming mini-fullerenes and their graphs // *Materials Phys. Mech*. **20** (2014) 1.
[96] A.I. Melker, S.A. Starovoitov, T.V. Vorobyeva, Classification of mini-fullerenes on graph basis // *Materials Phys. Mech*. **20** (2014) 12.
[97] A.I. Melker, M.A. Krupina, Designing mini-fullerenes and their relatives on graph basis // *Materials Phys. Mech*. **20** (2014) 18.
[98] M.A. Krupina, A.I. Melker, S.A. Starovoitov, T.V. Vorobyeva, Structure and graphs of midi-fullerenes // *Proceedings of NDTCS' 2015* **16** (2015) 23.
[99] K. Xia, X. Feng, Y. Tong, G.W. Wei, Persistent homology for the quantitative prediction of fullerene stability // *J. Comput. Chem*. **36** (2015) 408.
[100] P. Schwerdtfeger, L. N. Wirz, J. Avery, The topology of fullerenes // *WIREs Comput. Mol. Sci.* **5** (2015) 96. doi: 10.1002/wcms.1207
[101] D. Nicodemos, M. Stehlik, Fullerene graphs of small diameter, *arXiv*:1604.01934v1 [math.CO] 7 Apr 2016.
[102] A.I. Melker, *Dynamics of Condensed Matter, Vol. 1, Vibrations and Waves* (St. Petersburg Academy of Sciences on Strength Problems, 2013)
[103] A.I. Melker, T.V. Vorobyeva, R.M. Zarafutdinov, Structure and energy of Δn=6 series fullerenes // *Proceedings of NDTCS- 2017* **17** (2017) 75.
[104] A.I. Melker, M.A. Krupina, R.M. Zarafutdinov, Structure of Δn=10 series fullerenes // *Proceedings of NDTCS-2017* **17** (2017) 68.
[105] A.I. Melker, M.A. Krupina, R.M. Zarafutdinov, Periodic system for perfect fullerenes obtained by fusion reactions // *Proceedings of NDTCS-2017* **17** (2017) 72.
[106] A.I. Melker, T.V. Vorobyeva, R.M. Zarafutdinov, Structure and energy of Δn=14 series fullerenes // *Proceedings of NDTCS- 2017* **17** (2017) 79.
[107] A.I. Melker, On the nature of void swelling // *Proc. SPIE* **7377** (2008) 737710-1.
[108] F. Harary, *Graph Theory* (Addison-Wesley Publishing Co. Reading, 1969)