Materials Physics and Mechanics 20 (2014) 18-24 Received: April 29, 2014

DESIGNING MINI-FULLERENES AND THEIR RELATIVES ON GRAPH BASIS

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

[1]Department of Mechanics and Control Processes,

[2]Department of Experimental Physics,

St. Petersburg State Polytechnical University, Polytekhnicheskaya 29,

195251, St. Petersburg, Russia

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

Abstract. Different families of fullerenes taking as a basis their progenitors, mini-fullerenes, and graph theory were constructed. They are: a family of a bi-trefoil: C_{14}, C_{18}, C_{24}, C_{30}, $C_{36;}$ a family of truncated bipyramids: C_{14}, C_{18}, C_{24} C_{30}, C_{36}; a family of cupola half-fullerenes: C_{10}, C_{12}, C_{16}, C_{20}, C_{24}; and a family of 4-6-equator fullerenes: C_{20}, C_{24}, C_{32}, C_{40}, C_{48}. All the families contain five members and have a layer structure. By analogy with geography, we can distinguish two frigid zones composed of pentagons and a torrid zone composed of hexagons. The smallest fullerenes of each family are exceptions; its frigid zones are formed of squares. Another interesting feature is that the torrid zone in the family of 4-6-equator fullerenes: C_{20}, C_{24}, C_{32}, C_{40}, and C_{48} is composed of square-hexagon pairs. We have also constructed a family of cupola half-fullerenes: C_{10}, C_{12}, C_{16}, C_{20}, and C_{24}. with the help of transition to modified graphs introduced in [3], where a cluster of three or four atoms being considered as a big point (vertex) contrary to a zero-size point (vertex) of a common graph.

1. Introduction

In [1] the term "*fullerene*" was taken in a broad sense as 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 geometrical approach allowed obtaining possible forms of mini-fullerenes (from C_4 to C_{20}). The diagrams, describing the process of forming these fullerenes of single carbon atoms and carbon dimers, as well as of small carbon clusters, were considered elsewhere [2, 3]. But what is more important, we have constructed graphs for all the mini-fullerenes [2, 3]. The graph analysis simplifies an understanding of both the ways of fullerene forming and its structure. On the basis of the graphs it is possible to distinguish different families of mini-fullerenes and therefore to make a classification of these unusual carbon structures.

However, there is one obstacle, namely, how to present these structures. Graph presentation is very convenient for a mathematical analysis, but sometimes it is difficult for understanding. On the other hand, different types of axonometry allow us to gain a rough idea of these structures. Unfortunately, it is true mostly for fullerenes of small number of atoms. Besides, it is a very tedious procedure to build an axonometric image for fullerenes of large number of atoms. Luckily, there is a method which is using for a long time by tailors and children: cutting out a pattern. Strictly speaking, it is a type of a graph presentation, where everybody chooses one's own rules. In what is following, we will use, together with graphs and axonometry, cutting out a pattern in the similar manner as it was developed for scanning cyclohexane electronic structure [4].

In this contribution we have tried to solve the following problem; namely; how to construct new fullerenes designing its graphs, if one knows the graphs and atomic structure of mini-fullerenes. In [3] we included into any family only the members from C_4 to C_{20}. It was connected with the fact that we restricted ourselves with mini-fullerenes, which cannot contain more than twenty carbon atoms (according to our definition accepted at that time). Now we enlarge our consideration and will consider all the possible fullerenes which structures can be obtained on the basis of graphs, starting with the structures of mini-fullerenes.

2. Family of a bi-trefoil: C_{14}, C_{18}, C_{24}, C_{30}, C_{36}

In [3] only two members: a bi-shamrock (tetra$_6$-hexa$_3$ polyhedron) C_{14}, and a truncated bi-shamrock ((tri-penta$_3$)$_2$-hexa$_3$ polyhedron) C_{18} were included into this family. In Fig. 1 the full family is shown. It contains, beside a bi-trefoil and a truncated bi-trefoil, a bi-quatrefoil C_{24}, a bi-quinquefoil C_{30}, and a bi-sexfoil C_{36}.

The fullerenes have a layer structure. By analogy with geography, we can distinguish two frigid zones composed of pentagons and a torrid zone composed of hexagons. It should be mentioned that the smallest fullerene, C_{14}, is an exception. It is not truncated, so its frigid zones are formed of squares.

It should be emphasized that the central part of these graphs for truncated bi–polyfoils coincides with the graphs of the family of barrel-shaped fullerenes: C_{12}, C_{16}, C_{20}, C_{24} (see Fig. 5 in [3]).

3. Family of truncated bipyramids: C_{14}, C_{18}, C_{24} C_{30}, C_{36}

In [3] only two members: a base-truncated triangular bipyramid C_{14}, and a truncated triangular bipyramid C_{18} were included into this family. Now we are not restricted with mini-fullerenes. The full family is shown in Fig. 2. It contains also a truncated octahedron C_{24}, a truncated five-angle bipyramid C_{30}, and a truncated six-angle bipyramid C_{36}.

It should be emphasized that in Fig. 2 modified graphs are given. The point is that in [3] some innovations into the graph theory were done. Usually each vertex (point) of a graph corresponds to one atom. We suggested considering a cluster of three or four atoms as a big point (vertex) contrary to a zero-size point (vertex) of ordinary graphs. It allows do some operations with the new graphs in same manner as with a usual graph that simplifies an analysis. The modified graph gives a clearer insight into the structure of a fullerene.

The fullerenes have also a layer structure, but contrary to the previous family, now we have only two frigid zones composed of hexagons and no torrid zone. Here, as before, the smallest fullerene, C_{14}, is an exception; their frigid zones composed of pentagons.

4. Family of cupola half-fullerenes: C_{10}, C_{12}, C_{16}, C_{20}, C_{24}

This is a new family which is shown in Fig. 3 and which we have not noticed before. An understanding of its existence was reached after transition to modified graphs. The half-fullerenes similar to a half-sphere have only one zone, composed of either pentagons or hexagons.

5. Family of 4-6-equator fullerenes: C_{20}, C_{24}, C_{32}, C_{40}, C_{48}

This family is shown in Fig. 4. The progenitor C_{20} was constructed in [1], as an isomer of the smallest usual fullerene, a dodecahedron. The fullerenes have a layer structure: two frigid zones composed of pentagons and a torrid zone composed of pairs of square and hexagon. The smallest fullerene, a progenitor C_{20}, is an exception.

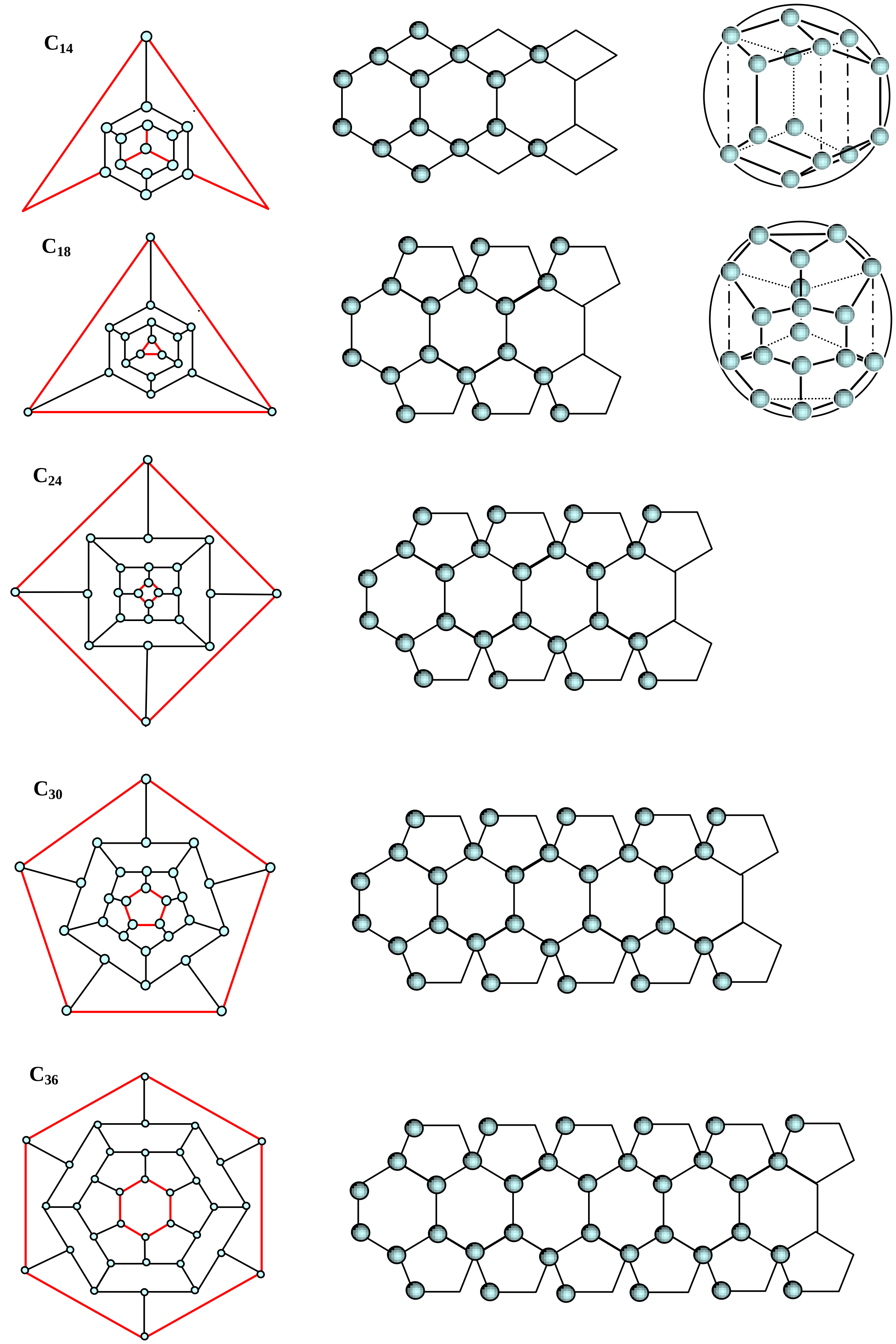

Fig. 1. Graphs of bi-polyfoils (on the left), its patterns (in the middle), and axonometric drawing of a bi-trefoil and a truncated bi-trefoil (on the right).

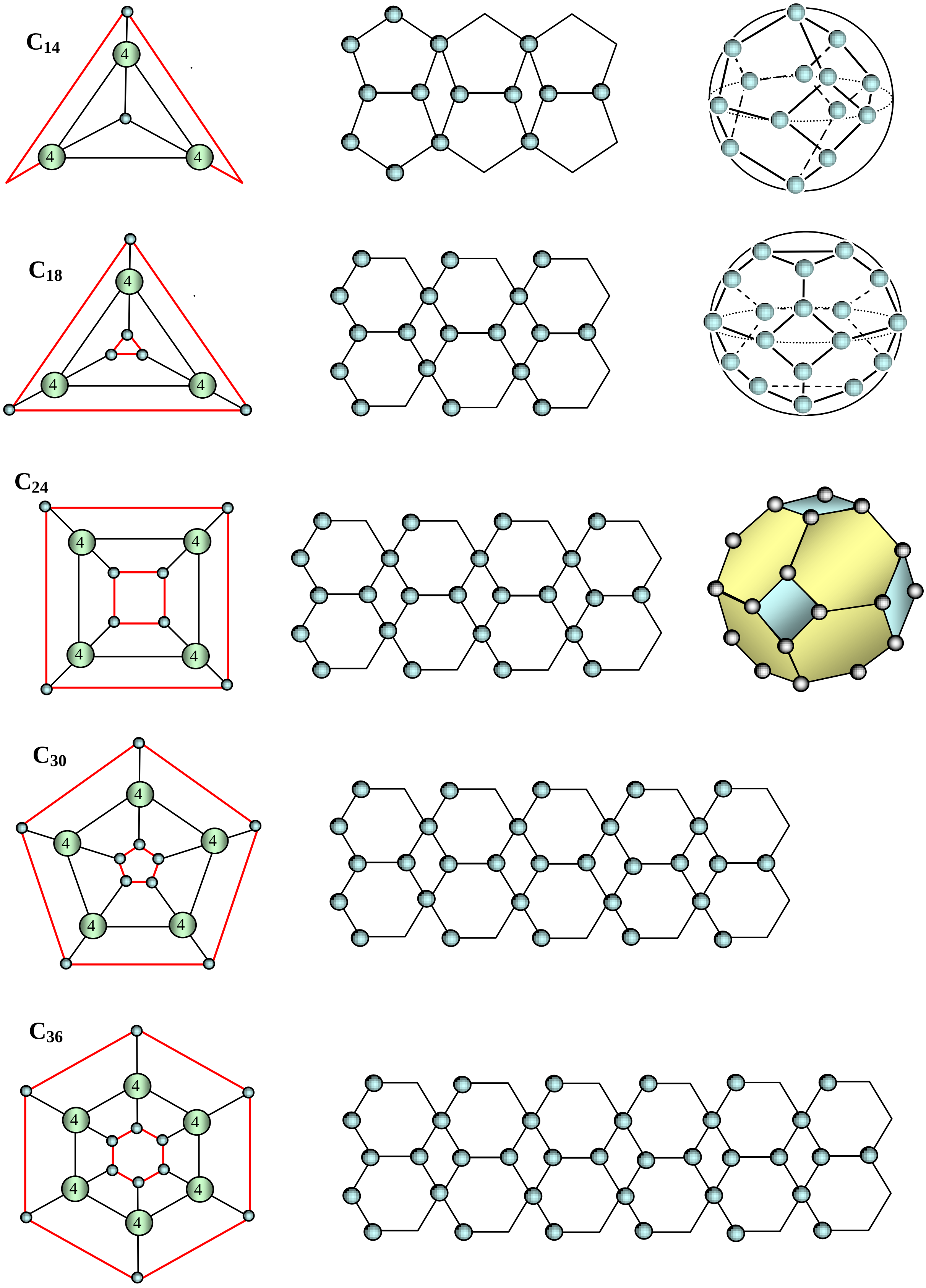

Fig. 2. Modified graphs of bipyramids (on the left), its patterns (in the middle), and axonometric drawing of a base-truncated triangular bipyramid, a truncated triangular bipyramid and a truncated octahedron (on the right).

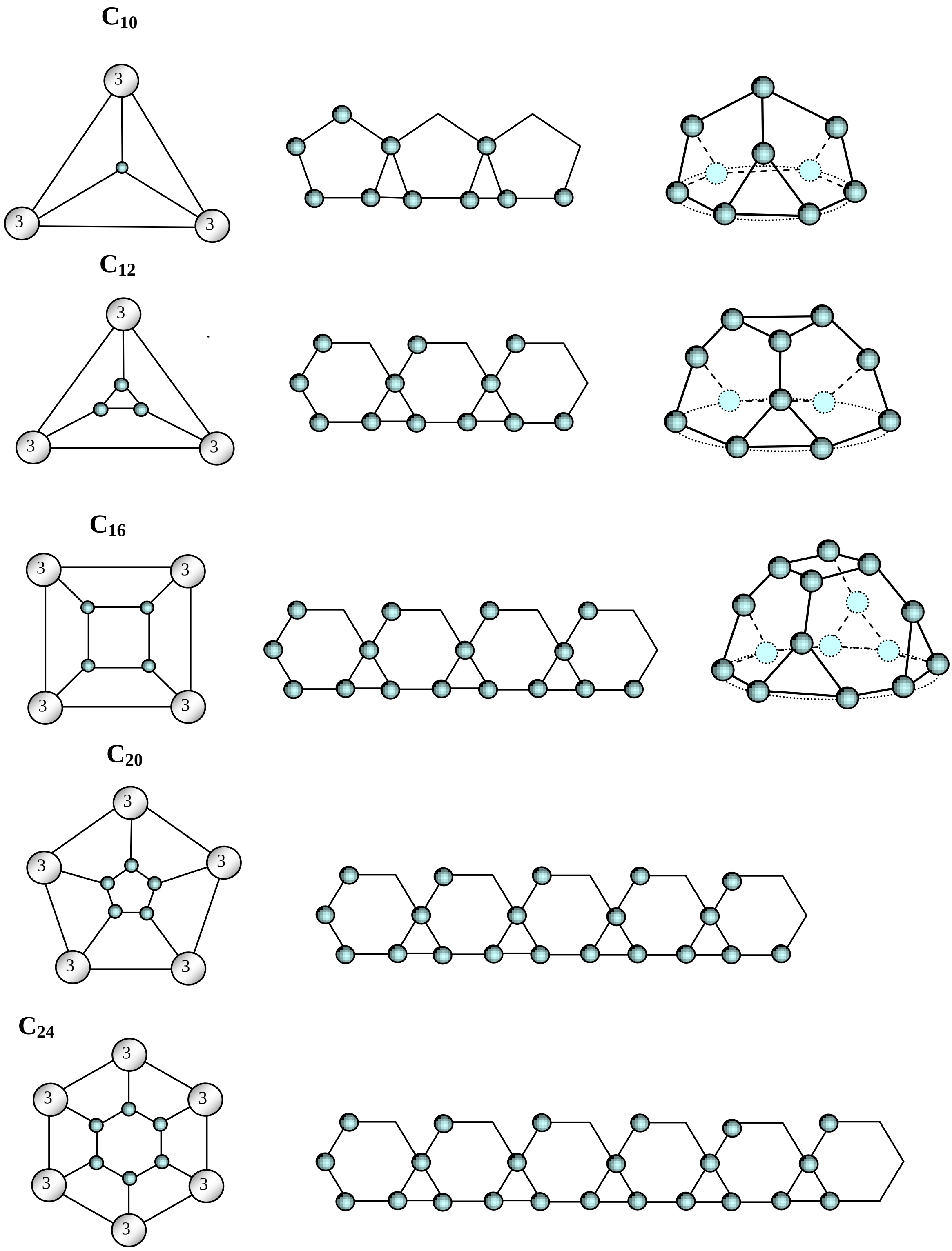

Fig. 3. Modified graphs of cupola half-fullerenes (on the left), its patterns (in the middle), and axonometric drawing of a base-truncated triangular pyramid, a truncated triangular pyramid, and a truncated tetra-angular pyramid (on the right).

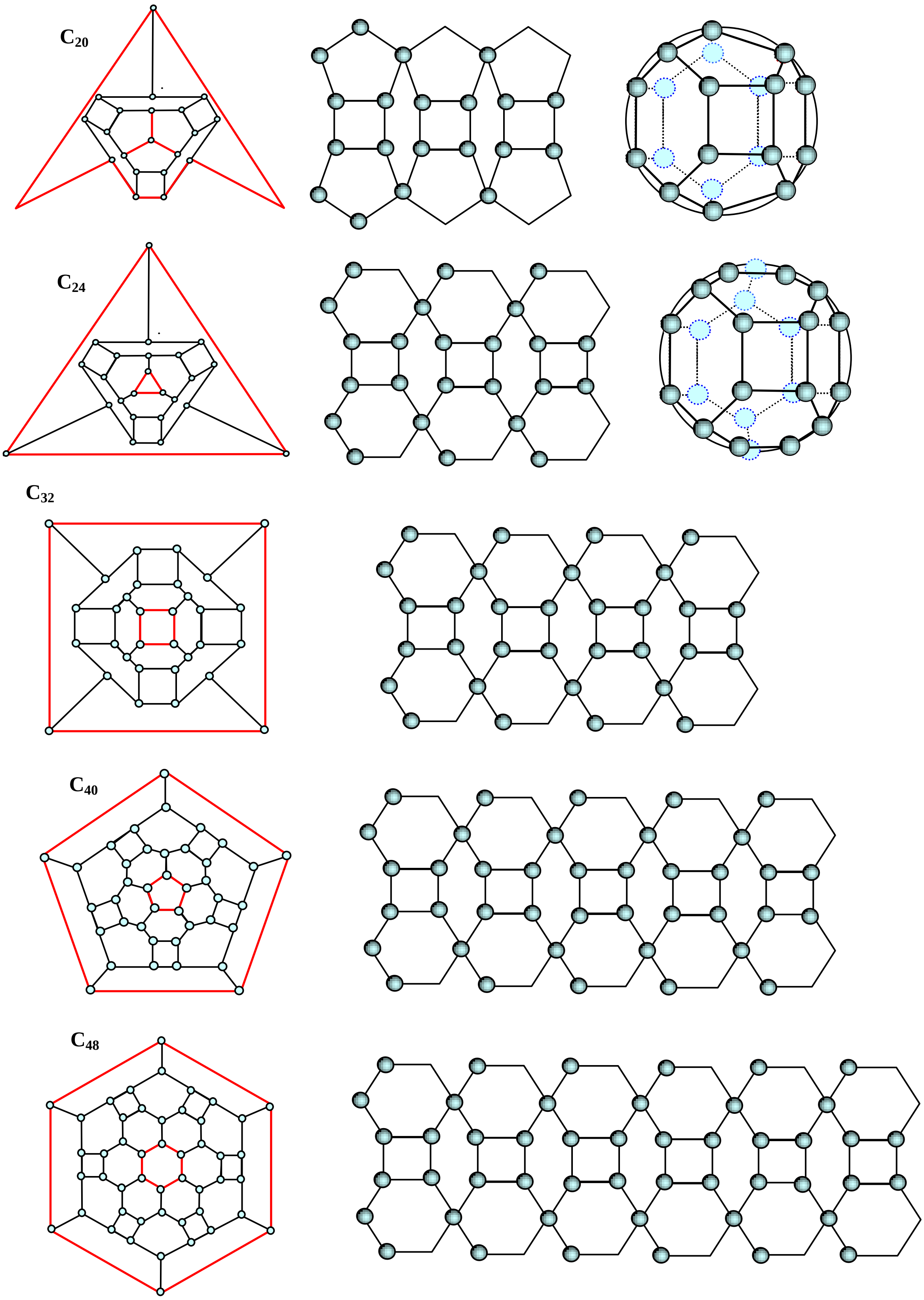

Fig. 4. Graphs of 4-6-equator fullerenes (on the left), its patterns (in the middle), and axonometric drawing of two first fullerenes (on the right).

6. Conclusion

We have constructed different families of fullerenes taking as a basis its progenitors, mini-fullerenes. All the families contain five members and have a layer structure. By analogy with geography, we can distinguish two frigid zones composed of pentagons and a torrid zone composed of hexagons. The smallest fullerenes of each family are exceptions; its frigid zones are formed of squares.

Another interesting feature is the structure of the torrid zone of the family of 4-6-equator fullerenes: C_{20}, C_{24}, C_{32}, C_{40}, $C_{48,}$ which composed of pairs of square and hexagon.

Besides, we have constructed a family of cupola half-fullerenes: C_{10}, C_{12}, C_{16}, C_{20}, C_{24}. An understanding of its existence was reached after transition to modified graphs introduced in [3], where a cluster of three or four atoms being considered as a big point (vertex) contrary to a zero-size point (vertex) of a common graph.

References

[1] A.I. Melker, V. Lonch // *Materials Physics and Mechanics* **13** (2012) 22.

[2] A.I. Melker // *Materials Physics and Mechanics* **20** (2014) 1.

[3] A.I. Melker, S.A. Starovoitov, T.V. Vorobyeva // *Materials Physics and Mechanics* **20** (2014) 12.

[4] A.I. Melker, M.A. Krupina // *Materials Physics and Mechanics* **9** (2010) 11.