

## MODELING GROWTH OF MIDI-FULLERENES FROM $C_{48}$ TO $C_{72}$

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**Abstract.** Axonometric projections together with corresponding graphs for tetra-hexa-cell-equator fullerenes are constructed in the range from 48 to 72. A unified approach for drawing axonometric projections of the fullerenes was used. The process of growth of fullerenes is studied on the basis of the mechanism, according to which a carbon dimer embeds in a hexagon of an initial fullerene. As a result, there arises a new atomic configuration and there is mass increase of two carbon atoms. We obtained direct descendents of the fifth branch of tetra-hexa-cell-equator family which begins with  $C_{48}$ ; namely  $C_{50}$ ,  $C_{52}$ ,  $C_{54}$ ,  $C_{56}$ ,  $C_{58}$ ,  $C_{60}$ ,  $C_{62}$ ,  $C_{64}$ ,  $C_{66}$ ,  $C_{68}$ ,  $C_{70}$ , and  $C_{72}$ . Among them only three fullerenes,  $C_{48}$ ,  $C_{60}$  and  $C_{72}$  are highly symmetric. The symmetry can be easily discovered looking at their graphs. On the basis of this study, as well as previous investigations the periodic system of fullerenes is suggested.

**Keywords:** carbon dimer, fullerene, graph, modeling, structure.

### 1. Introduction

Most investigations of fullerenes and nanotubes have centered on either obtaining these materials experimentally or studying properties of the materials which structure was usually postulated. To our mind, the crucial questions for advanced applications of these materials are: how the materials are originated and what structure they obtain.

Up to now mechanism of fullerene- and nanotube-formation is a controversial point. Many different models have been proposed to explain their formation. 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 [1-10]. In the second case, fullerenes and nanotubes are thought as direct transformation of graphene into fullerenes or nanotubes [11-17].

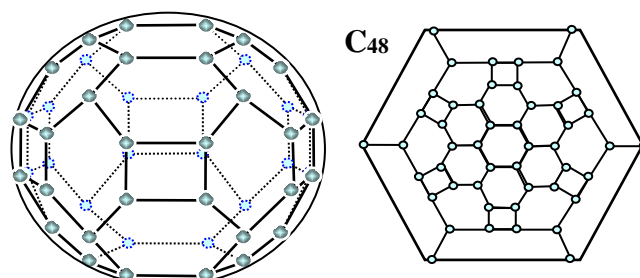
We will follow to one of the first-group mechanisms suggested for the first time in [1] because it has better justification [4]. Besides, it allows classify fullerene structures [8]. Briefly, it consists in the following. A carbon dimer embeds into a hexagon of an initial fullerene. As a result, instead of the hexagon adjoining two pentagons, when the dimer embeds into this hexagon, one obtains two adjacent pentagons adjoining two hexagons; there arises a new atomic configuration and there is mass increase of two carbon atoms

In doing so, we geometrically modeled growth of the second branch of the family of tetra-hexa-cell equator fullerenes beginning with  $C_{24}$  [8] in the range from 24 to 48. We have constructed the axonometric projections and the corresponding graphs for these fullerenes.

In this contribution we consider direct descendents of the tetra-hexa-cell-equator family of fullerenes from  $C_{48}$  to  $C_{72}$ . Our aim is at first to obtain their graphs, what is simpler, and then to construct the structure of fullerenes on the basis of the graphs obtained.

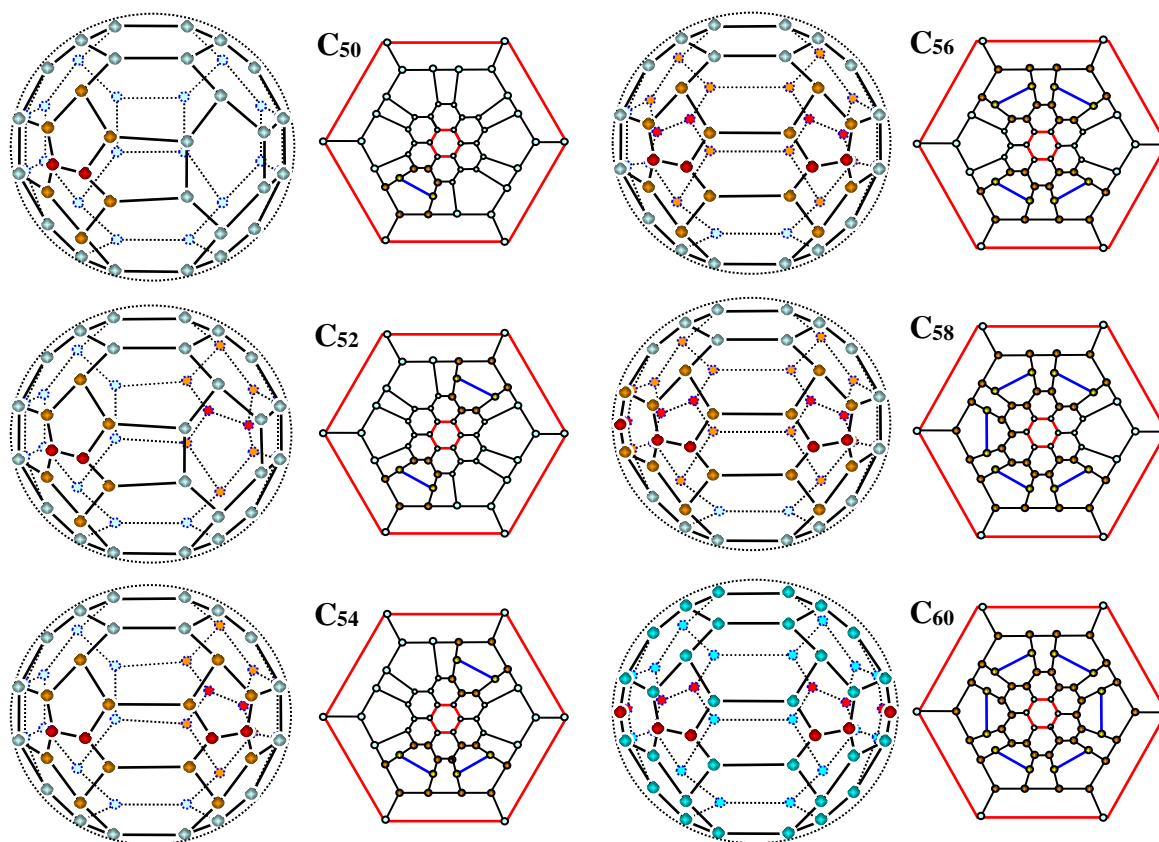
## 2. Growth of tetra<sub>6</sub>-hexa<sub>20</sub> polyhedral fullerene C<sub>48</sub>

The atomic configuration of this fullerene consists of six squares and twenty hexagons, so it was named a tetra<sub>6</sub>-hexa<sub>20</sub> polyhedron. Its structure can be composed of two cupola half-fullerenes C<sub>24</sub>; each of them has in its center a hexagon being surrounded with six hexagons. The cupolas can react with each other [11] creating two isomers of fullerene C<sub>48</sub>, one of which having  $D_{6h}$  symmetry is shown in Figure 1.



**Fig. 1.** Atomic structure and graph of a tetra<sub>6</sub>-hexa<sub>20</sub> polyhedron C<sub>48</sub>.

**First stage.** Starting with this fullerene, one can obtain its direct descendants through the use of dimer embedding into a hexagon. We have emphasized in our previous papers that drawing the axonometric projections of fullerenes is a rather tedious procedure, but it allows avoiding many mistakes in subsequent reasoning. Constructing the fullerene graphs is easier than drawing the axonometric projections. Taking as a basis the structure and graph of fullerene C<sub>48</sub>, we have obtained the fullerenes from C<sub>48</sub> to C<sub>60</sub> (Fig. 2). To gain a better understanding of the mechanism of dimer embedding, its main features are given in the form of scheme (Fig. 3).



**Fig. 2.** Atomic structure and graphs of some fullerenes C<sub>50</sub>, C<sub>52</sub>, C<sub>54</sub>, C<sub>56</sub>, C<sub>58</sub>, and C<sub>60</sub>.

Let us analyze these figures. From the configurations shown it follows that the first embedding transforms fullerene C<sub>48</sub> into fullerene C<sub>50</sub>. It influences deeply only on one of hexagons and two its square neighbors. The hexagon transforms into two adjacent pentagons and its square neighbors become pentagons; the whole fullerene losing six-fold symmetry. As a consequence, there arises a cell which contains four pentagons.

The second imbedding transforms fullerene C<sub>50</sub> into fullerene C<sub>52</sub>. It can be done by two ways. As a result one obtains two isomers having different symmetry. Similar to the previous case, in the fullerene having  $D_{1h}$  symmetry one of nearest to the cell hexagons transforms into two adjacent pentagons, its square neighbor into a pentagon, and its pentagon neighbor into a hexagon (growth from one nucleus). Other isomer contains two isolated cells of four pentagons (growth from two nuclei).

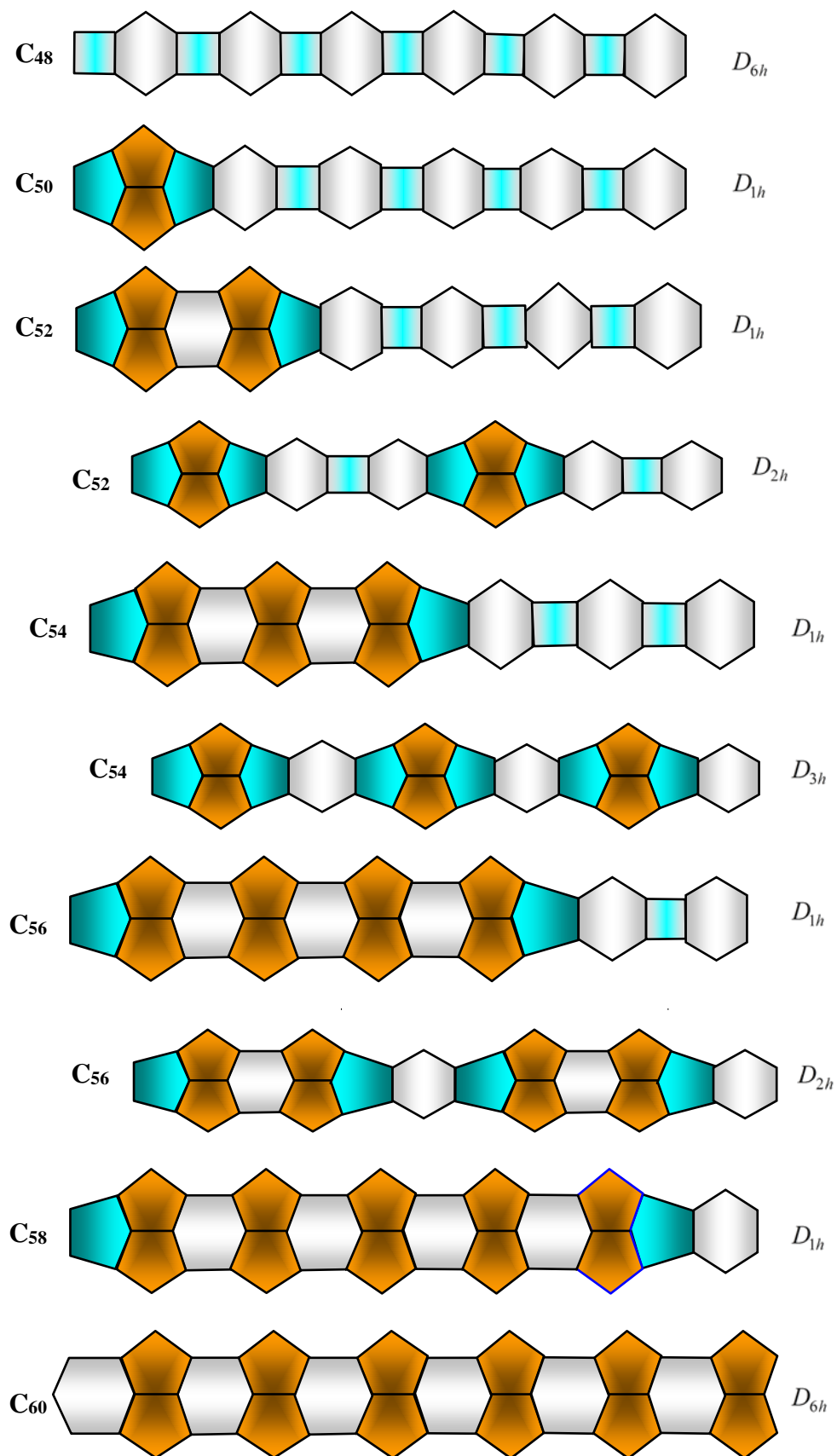
The third embedding leads to transition from fullerene C<sub>52</sub> to fullerene C<sub>54</sub>. In the case of one-nucleus growth it eliminates one more hexagon and two its neighbors, a pentagon and a square, but in return creates an adjacent hexagon of another local orientation and a new pentagon. It is possible also to obtain several different isomers; one of them having  $D_{3h}$  symmetry is shown in Figure 3.

The fourth imbedding transforms fullerene C<sub>54</sub> into fullerene C<sub>56</sub>; two isomers are presented in Figure 3. The fifth embedding changes fullerene C<sub>56</sub> into fullerene C<sub>58</sub>. At last the sixth embedding which leads to fullerene C<sub>60</sub> restores the six-fold symmetry. The fullerene C<sub>60</sub> obtained could be named hexa-octa-cell-equator fullerene where every two adjacent pentagons have the form of a bow tie (see the scheme at the bottom of Figure 3).

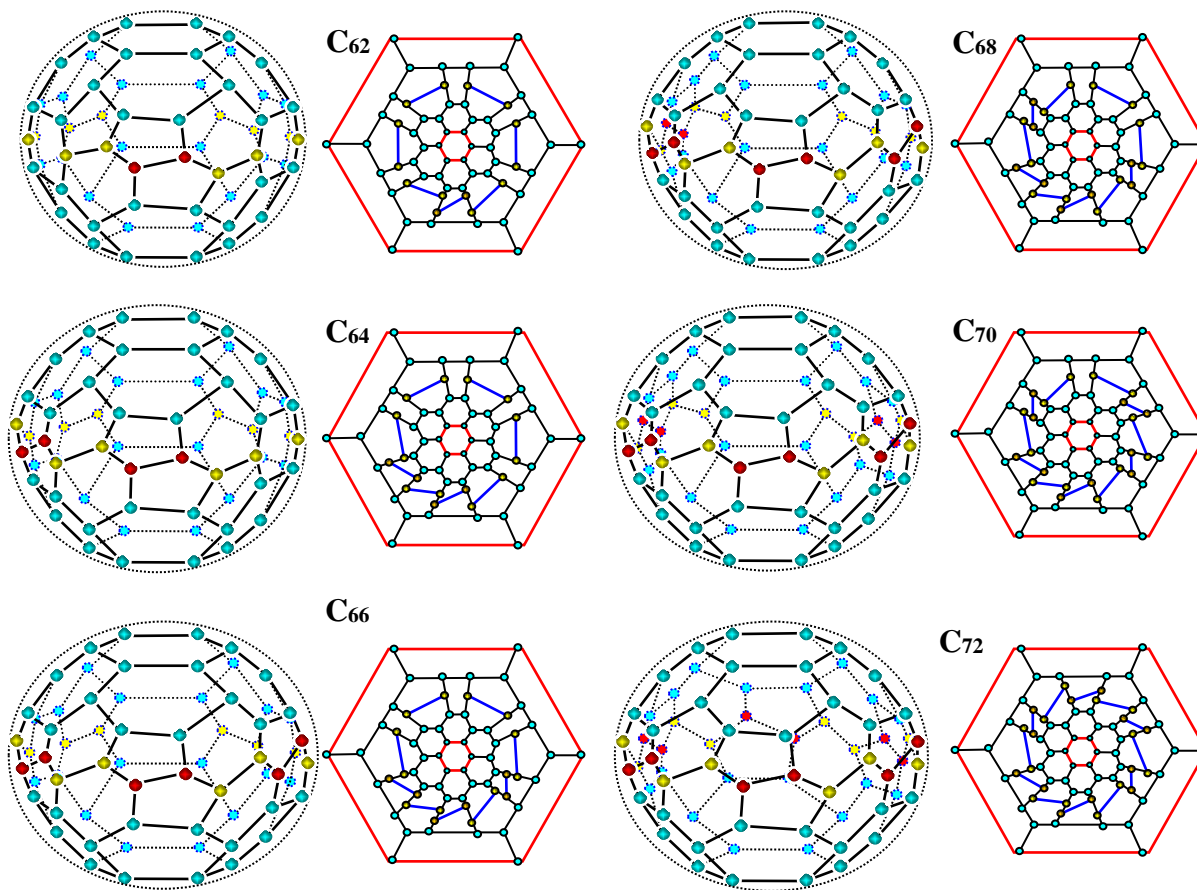
**Second stage.** Now the fullerene C<sub>60</sub> is up against the problem; it can grow only at an angle to its axes of symmetry. It is connected with the fact that embedding can be realized only normal to a direction along which a hexagon has two neighboring mutually antithetic pentagons. During the further growth by dimer embedding, one obtains fullerenes C<sub>62</sub>, C<sub>64</sub>, C<sub>66</sub>, C<sub>68</sub>, C<sub>70</sub>, and C<sub>72</sub> (Fig. 4). The structure of fullerene C<sub>72</sub> is rather interesting. It is formed from six pairs of two adjacent pentagons along the equator separated with six pairs of two adjacent hexagons. To gain a better understanding of this structure, the pentagon pairs are specially marked in Figure 5. The main features of dimer embedding are given in the form of schematic representation in Figure 6. We consider here only the growth from one nucleus. However, similarly to the first stage one can obtain many intermediate fullerenes having different symmetry.

### 3. Conclusion

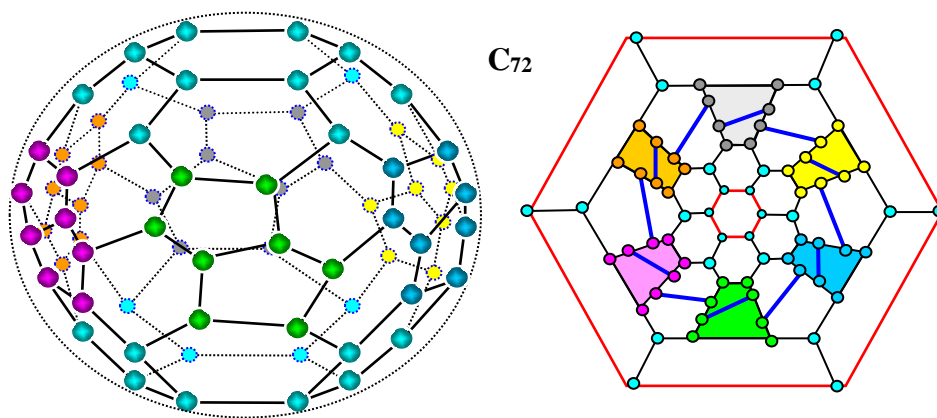
Axonometric projections together with corresponding graphs for tetra-hexa-cell-equator fullerenes are constructed in the range from 48 to 72. A unified approach for drawing axonometric projections of the fullerenes was used. It consists in the following; one should use the dimetric representation which symmetry coincides with that of a corresponding graph. The growth of fullerenes is studied on the basis of the mechanism, according to which a carbon dimer embeds in a hexagon of an initial fullerene. This leads to stretching and breaking the covalent bonds which are parallel to arising tensile forces. In this case, instead of the hexagon adjoining two pentagons, one obtains two adjacent pentagons adjoining two hexagons. As a result, there arises a new atomic configuration and there is mass increase of two carbon atoms. We obtained direct descendents of the fifth branch of the tetra-hexa-cell-equator family 6 which begins with C<sub>48</sub>; namely C<sub>50</sub>, C<sub>52</sub>, C<sub>54</sub>, C<sub>56</sub>, C<sub>58</sub>, C<sub>60</sub>, C<sub>62</sub>, C<sub>64</sub>, C<sub>66</sub>, C<sub>68</sub>, C<sub>70</sub>, and C<sub>72</sub>. Among them only three fullerenes, C<sub>48</sub>, C<sub>60</sub> and C<sub>72</sub> are highly symmetric. The symmetry can be easily discovered looking at their graphs.



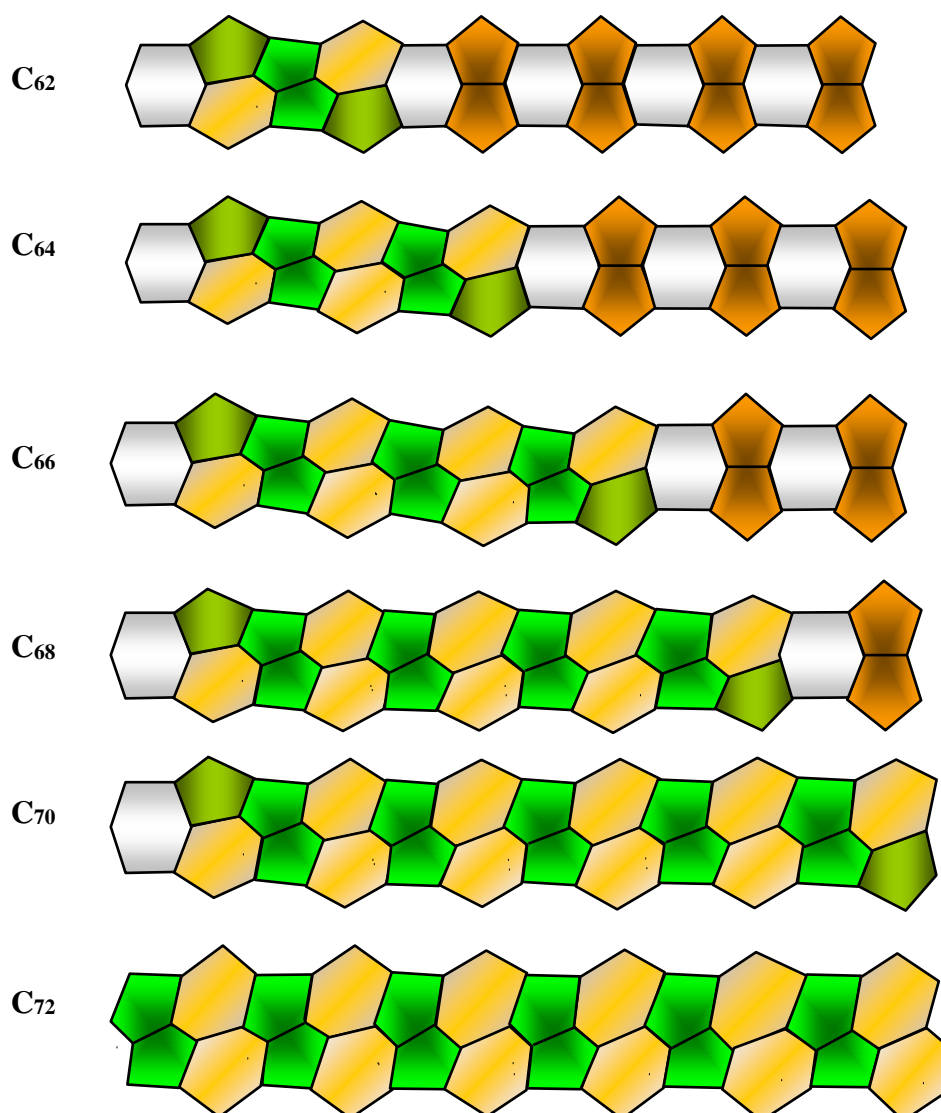
**Fig. 3.** Scheme reflecting the main structural changes during the growth of fullerene C<sub>50</sub>.



**Fig. 4** Atomic structure and graphs of some fullerenes  $C_{62}$ ,  $C_{64}$ ,  $C_{66}$ ,  $C_{68}$ ,  $C_{70}$ , and  $C_{72}$ .



**Fig. 5.** Six in-pairs-adjacent pentagons in fullerene  $C_{72}$ .



**Fig. 6.** Scheme reflecting the main structural changes during the growth of fullerene  $C_{62}$ .

#### 4. Discussion

In the Introduction, we have set off for fullerenes the crucial questions from the rest ones; namely, how the fullerenes are originated and what structure they obtain naturally. However, the most important and most difficult question for any science is classification [18]. Let us consider what can be done in this regard for fullerenes.

Modeling the growth of fullerenes from  $C_{24}$  ( $D_{3h}$  symmetry) to  $C_{48}$ , we have obtained the perfect fullerenes  $C_{30}$  and  $C_{36}$  conserving three-fold symmetry [8]. Modeling the growth of fullerenes from  $C_{32}$  ( $D_{4h}$  symmetry) to  $C_{60}$ , we found perfect fullerenes  $C_{40}$  and  $C_{48}$  conserving four-fold symmetry [9]. Modeling the growth of fullerenes from  $C_{40}$  ( $D_{5h}$  symmetry) to  $C_{68}$ , we found perfect fullerenes  $C_{50}$  and  $C_{60}$  conserving five-fold symmetry [10]. In this study, starting from fullerene  $C_{48}$  ( $D_{6h}$  symmetry), we have obtained perfect fullerenes  $C_{60}$  and  $C_{72}$ . The mass difference between successive fullerenes in the first case is  $\Delta m=6$ , in the second case  $\Delta m=8$ , in the third case  $\Delta m=10$  and in the fourth case  $\Delta m=12$ . It should be emphasized that in all the cases the mass difference is equal to a double degree of symmetry. On the basis of these investigations, as well as others, we can submit the following periodic system for embedded fullerenes. It should be mentioned that preliminary sketches of the periodic system are given in Refs. [10, 19].

### Periodic System of Fullerenes

Symmetry of Fullerenes				
3-fold S $\Delta m=6$	3-fold T $\Delta m=6$	4-fold $\Delta m=8$	5-fold $\Delta m=10$	6-fold $\Delta m=12$
<b>C<sub>14</sub></b> C <sub>16</sub> C <sub>28</sub>	<b>C<sub>18</sub></b> C <sub>20</sub> C <sub>22</sub>	<b>C<sub>24</sub></b> C <sub>26</sub> C <sub>28</sub> C <sub>30</sub>	<b>C<sub>30</sub></b> C <sub>32</sub> C <sub>34</sub> C <sub>36</sub> C <sub>38</sub>	<b>C<sub>36</sub></b> C <sub>38</sub> C <sub>40</sub> C <sub>42</sub> C <sub>44</sub> C <sub>46</sub>
<b>C<sub>20</sub></b> C <sub>22</sub> C <sub>24</sub>	<b>C<sub>24</sub></b> C <sub>26</sub> C <sub>28</sub>	<b>C<sub>32</sub></b> C <sub>34</sub> C <sub>36</sub> C <sub>38</sub>	<b>C<sub>40</sub></b> C <sub>42</sub> C <sub>44</sub> C <sub>46</sub> C <sub>48</sub>	<b>C<sub>48</sub></b> C <sub>50</sub> C <sub>52</sub> C <sub>54</sub> C <sub>56</sub> C <sub>58</sub>
<b>C<sub>26</sub></b> C <sub>28</sub> C <sub>30</sub>	<b>C<sub>30</sub></b> C <sub>32</sub> C <sub>34</sub>	<b>C<sub>40</sub></b> C <sub>42</sub> C <sub>44</sub> C <sub>46</sub>	<b>C<sub>50</sub></b> C <sub>52</sub> C <sub>54</sub> C <sub>56</sub> C <sub>58</sub>	<b>C<sub>60</sub></b> C <sub>62</sub> C <sub>64</sub> C <sub>66</sub> C <sub>68</sub> C <sub>70</sub>
<b>C<sub>32</sub></b> C <sub>34</sub> C <sub>36</sub>	<b>C<sub>36</sub></b> C <sub>38</sub> C <sub>40</sub>	<b>C<sub>48</sub></b> C <sub>50</sub> C <sub>52</sub> C <sub>54</sub>	<b>C<sub>60</sub></b> C <sub>62</sub> C <sub>64</sub> C <sub>66</sub> C <sub>68</sub>	<b>C<sub>72</sub></b> C <sub>74</sub> C <sub>76</sub> C <sub>78</sub> C <sub>80</sub> C <sub>82</sub>
<b>C<sub>38</sub></b> C <sub>40</sub> C <sub>42</sub>	<b>C<sub>42</sub></b> C <sub>44</sub> C <sub>46</sub>	<b>C<sub>56</sub></b> C <sub>58</sub> C <sub>60</sub> C <sub>62</sub>	<b>C<sub>70</sub></b> C <sub>72</sub> C <sub>74</sub> C <sub>76</sub> C <sub>78</sub>	<b>C<sub>84</sub></b> C <sub>86</sub> C <sub>88</sub> C <sub>90</sub> C <sub>92</sub> C <sub>94</sub>
<b>C<sub>44</sub></b> C <sub>46</sub> C <sub>48</sub>	<b>C<sub>48</sub></b> C <sub>50</sub> C <sub>52</sub>	<b>C<sub>64</sub></b> C <sub>66</sub> C <sub>68</sub> C <sub>70</sub>	<b>C<sub>80</sub></b> C <sub>82</sub> C <sub>84</sub> C <sub>86</sub> C <sub>88</sub>	<b>C<sub>96</sub></b> C <sub>98</sub> C <sub>100</sub> C <sub>102</sub> C <sub>104</sub> C <sub>106</sub>
<b>C<sub>50</sub></b>	<b>C<sub>54</sub></b>	<b>C<sub>72</sub></b>	<b>C<sub>90</sub></b>	<b>C<sub>108</sub></b>

All the fullerenes form five vertical columns (groups), having different symmetry. Two groups of three-fold symmetry differ by the structure of their apices. The 3-fold-symmetry group S has two sharp apices, the third-order axis going through them. The 3-fold-symmetry group T has two truncated apices, the third-order axis going through the centers of triangles. We suppose that the fullerenes of one and the same group have similar physical and chemical properties.

Strictly speaking, only the fullerenes denoted by bold symbols have the symmetry of a corresponding column. They are ideal (perfect) fullerenes. The others are imperfect or semi-perfect. As noted in Ref. [8] by analogy with crystal physics, the imperfection is connected with extra ‘interstitial’ dimers, playing the role of defects. Let us continue this analogy. In real crystals a long-range order is impossible in strict sense of the word, because of such defects as dislocations which violate translational symmetry. Nevertheless, the long-range order is observed experimentally, but this order is defined otherwise and is referred to as *topological long-range order* [19]. Following this example, we define the imperfect fullerenes conserving the main symmetry axis as having *topological symmetry*.

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