

CLASSIFICATION OF MINI-FULLERENES ON GRAPH BASIS

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Abstract. The diagrams, describing the process of forming mini-fullerenes (from C_4 to C_{20}) of single carbon atoms and carbon dimers, were suggested by one of the authors elsewhere. In this contribution we solved an inverse problem, i.e. how to predict possible ways of forming mini-fullerenes, if one knows its graphs. We have analyzed the graphs describing the process of forming mini-fullerenes and found that they can be formed not only of single carbon atoms and carbon dimers but also of small carbon clusters. On the basis of the graphs it is possible to distinguish different families of mini-fullerenes and therefore one can make a classification of these unusual carbon structures. In the course of the analysis some innovation to the graph theory was done. We suggested considering a cluster of three or four atoms as a big point (vertex) contrary to a zero-size point (vertex) of a common graph. In this case one obtains a graph, which is identical to a simpler graph. It allows do some operations with this graph in same manner as with a usual graph that simplifies an analysis.

1. Introduction

In [1] we have taken the term “*fullerene*” 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 us to obtain possible forms of such broad-sense fullerenes. To gain a more penetrating insight into its nature, we also have taken into consideration, along with the atomic structure of these spherical molecules, its electronic structure [2]. For this purpose we have developed an enlarged version of Sidgwick–Powell theory [3]. The modified version [4] was applied at first to cyclohexane [4] and usual fullerenes [5], and thereafter to the broad-sense fullerenes [1].

Up to now mechanism of fullerene formation is unclear. However, it is known that, if to take one electrode of ${}_6C^{13}$ –graphite and another of ordinary ${}_6C^{12}$ –graphite, the fullerene, formed in an electric arc, has ${}_6C^{13}$ – and ${}_6C^{12}$ – atoms arranged on a fullerene surface in a random way. This suggests that fullerene assemblage originates of separate atoms and C_2 –dimers, and probably of very small clusters. In [6, 7] this fact was used for postulating the ways of forming broad-sense fullerenes. Their final configurations were given not only in the usual form but in the form of graphs as well.

In this contribution we solved an inverse problem, i.e. how to predict possible ways of forming the broad-sense fullerenes, if one knows its graphs.

2. Tetrahedral fullerene C_4 as an explanation of some notions of the graph theory

In Fig. 1 two graphs representing a tetrahedron are shown (*a*, *b*). One can easily associate graph (*a*) with forming a tetrahedral fullerene initiated by a reaction-active single atom. Graph (*b*) displays forming it starting at a dimer. Nevertheless both graphs, having four vertices and six edges, are isomorphic. Remember that according to the graph theory [8], edges having a common vertex are named adjacent. Graphs having one-to-one correspondence and conserving the adjacency are isomorphic. Besides, both graphs are planar because they can be placed on a plane.

However, graph (*a*) resembles better a tetrahedron than more abstract graph (*b*). It is connected with the fact that in the first case an observer looks at a triangular pyramid (tetrahedron) from above. In the second case, a point of observation is located on a normal to skew edges. In the first case no two edges of a graph intersect and planar graph (*a*) is a plane one. A plane graph takes into account symmetry of a corresponding polyhedron better, and therefore it reflects better polyhedron structure, thus allowing gaining a more penetrating insight into its nature. To gain a better understanding, we will use in what follows mostly plane graphs. On the basis of graph similarity we can distinguish graph families.

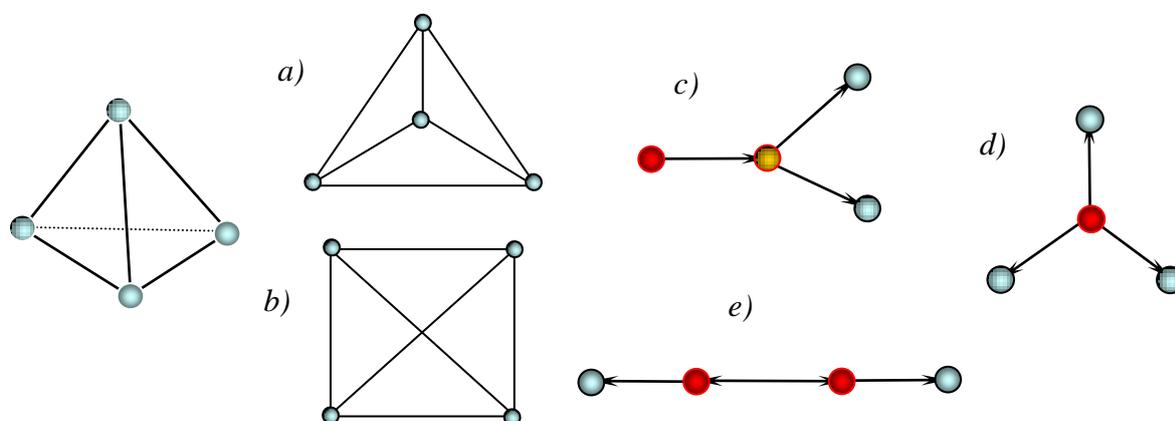


Fig. 1. Carbon tetrahedron (on the left) and two graphs (*a*, *b*) representing a tetrahedral fullerene. Graph (*b*) is planar because it is isomorphic to plane graph (*a*). Possible ways of forming a cluster of four carbon atoms (*c*, *d*, and *e*) are shown on the right.

3. Family of elementary fullerenes: from C_4 to C_{12}

This family of fullerenes will be named the elementary fullerenes. It contains together with a tetrahedron five members. In Fig. 2 the plane graphs of this family are shown. Looking at the figure, one can propose the ways of forming these carbon fullerenes which are quite different of those discussed in [6, 7]. They are illustrated in Fig. 3.

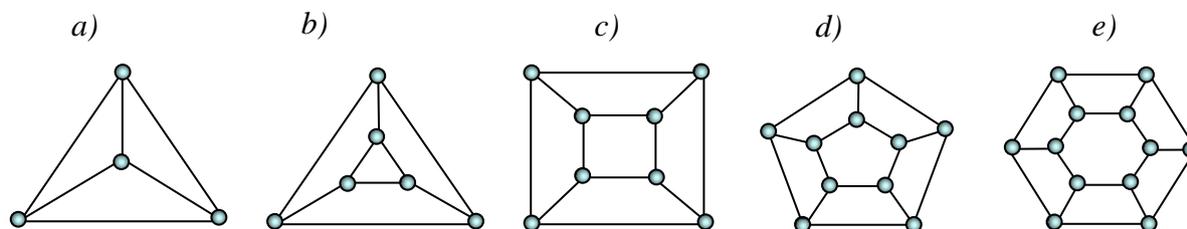


Fig. 2. Graphs: tetrahedron (*a*), triangular prism (*b*), cube (*c*), pentagonal prism (*d*), and hexagonal prism (*e*).

This suggests that fullerene assemblage originates not only of separate atoms and dimers, but also of very small clusters. This is not strange, since there are known such carbon

being the same as before. The ways of forming these carbon fullerenes are illustrated in Fig. 6. The structure of these fullerenes is given in Fig. 7.

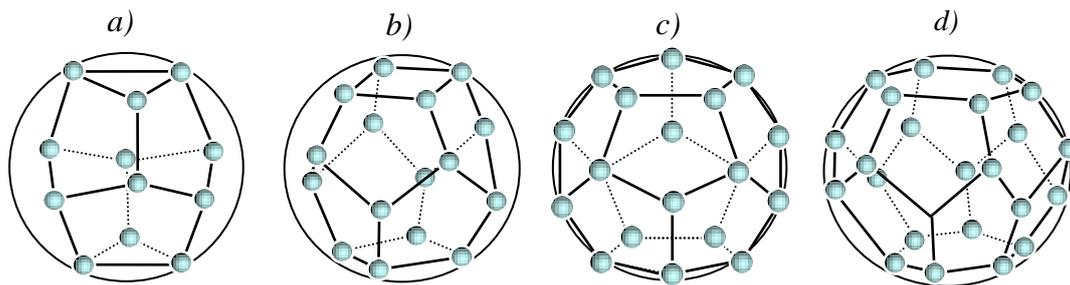


Fig. 7. Barrel-shaped fullerenes: triangular (*a*), square (*b*), five-cornered (*c*), six-cornered (*d*).

5. Truncated elementary fullerenes: C_{10} , C_{12} , C_{16}

This family contains three members, a base-truncated triangular pyramid, a truncated tetrahedron, and a half-truncated cube. Consider at first a truncated tetrahedron.

a) Truncated tetrahedron as an explanation of some innovation to the graph theory. In Fig. 8 different presentations of a truncated tetrahedron are given. Fig. 8a shows its graph. In much the same manner as for a triangular prism and a triangular barrel (Figs. 3b and 6a), one can mark out a reaction-active cluster of three atoms which initiates forming a truncated tetrahedron (Fig. 8b). Now the innovations. Up to now each vertex (point) of a graph corresponded to one atom. Now let us consider each cluster of three atoms as a big point (vertex) contrary to a zero-size point (vertex) of all the previous graphs. In this case we obtain a graph (Fig. 8c), which is identical to the graph of a tetrahedron (Fig. 1a). It allows do some operations with this graph in same manner as with a usual graph that simplifies an analysis. The atomic structure of this fullerene is given in Fig. 8d.

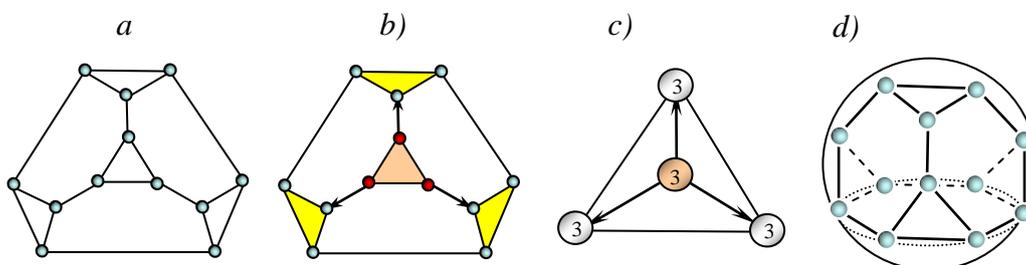


Fig. 8. Truncated tetrahedron fullerene: its graph (*a*), forming (*b*), reducing to a common tetrahedron (*c*), and its atomic structure (*d*).

b) Base-truncated triangular pyramid. Analogously we can analyze the formation and properties of a base-truncated triangular pyramid. At first we have a graph (Fig. 9a).

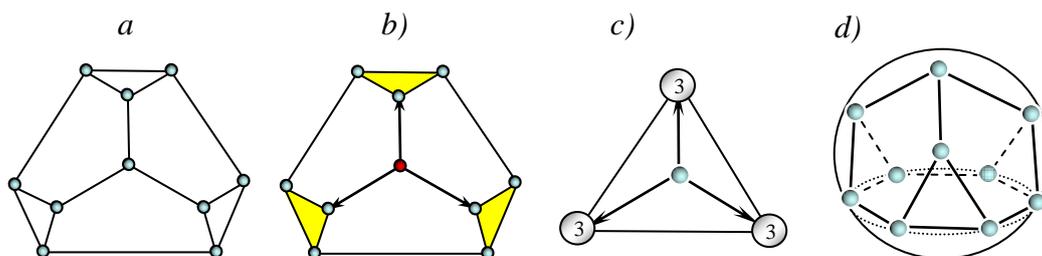


Fig. 9. Base-truncated triangular pyramid: its graph (*a*), coloring of blocks (*b*), and replacement of blocks by big vertices (*c*); its atomic structure (*d*).

Thereafter we find the clusters of three atoms (Fig. 9b), then change them with big points (Fig. 9c). As a result, we obtain the graph, although with two types of points (vertices), but which structure is simpler (Fig. 9d).

b) Half-truncated cube. Analogously we can analyze the formation and properties of a half-truncated cube. At first we have a graph (Fig. 10a). Thereafter we find the clusters of three atoms (Fig. 10b), then change them with big points (Fig. 10c). As a result, we obtain the graph, although with two types of points (vertices), but which structure is simpler and hence more convenient for analysis than that of the initial graph, to say nothing of the atomic structure (Fig. 10d).

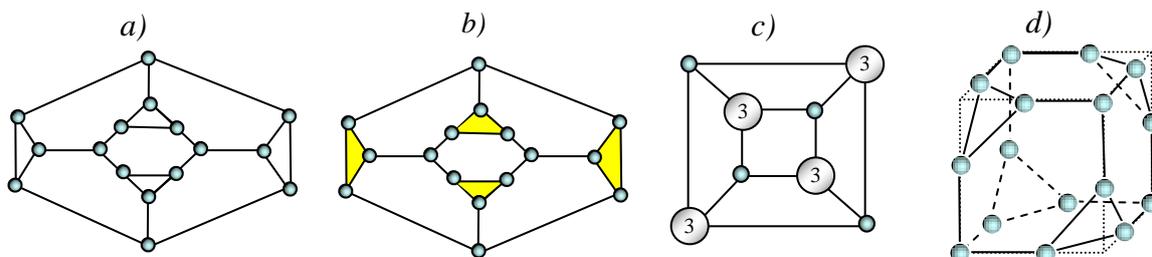


Fig. 10. Half-truncated cube: its graph (a), coloring of blocks (b), and replacement of blocks by big vertices (c); its atomic structure (d).

6. Truncated bipyramids: C_{14} , C_{18}

This family of fullerenes contains two members.

a) Base-truncated triangular bipyramid. In Fig. 11 different presentations of a base-truncated triangular bipyramid are given. Figure 11a shows its graph. In the same manner as before, one can mark out clusters of four atoms (Fig. 11b), and consider each cluster as a big point (vertex) (Fig. 11c). It allows also do some operations with this graph in same manner as with a usual graph. The atomic structure of this fullerene is given in Fig. 11d.

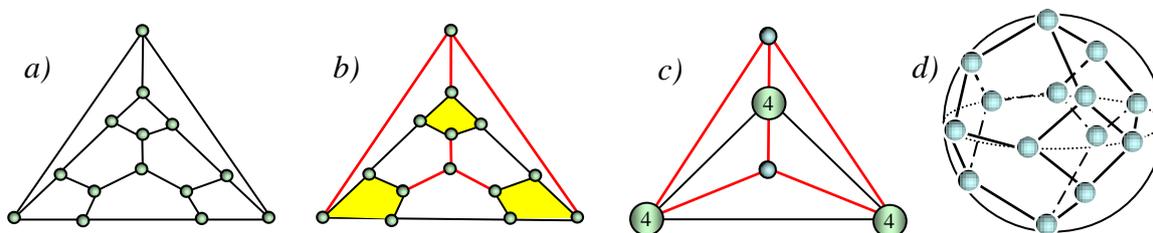


Fig. 11. Base-truncated triangular bipyramid: its graph (a), coloring of blocks (b), and replacement of blocks by big vertices (c); its atomic structure (d).

b) Truncated triangular bipyramid. Different presentations of a truncated triangular bipyramid are shown in Fig. 12. The following procedure has much in common with that of a base-truncated triangular bipyramid.

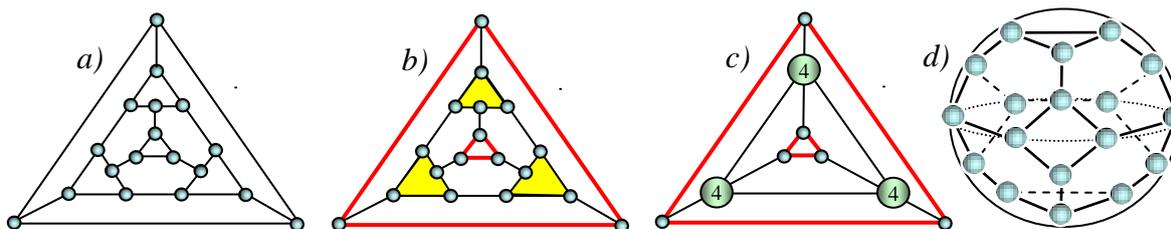


Fig. 12. Truncated triangular bipyramid: its graph (a), coloring of blocks (b), and replacement of blocks by big vertices (c); and its atomic structure (d).

7. Bi-shamrocks: C_{14} , C_{18}

This fullerene family contains two members: a bi-shamrock (tetra₆-hexa₃ polyhedron) and a truncated bi-shamrock ((tri-penta₃)₂-hexa₃ polyhedron). Its graphs and atomic structures are shown in Fig. 13.

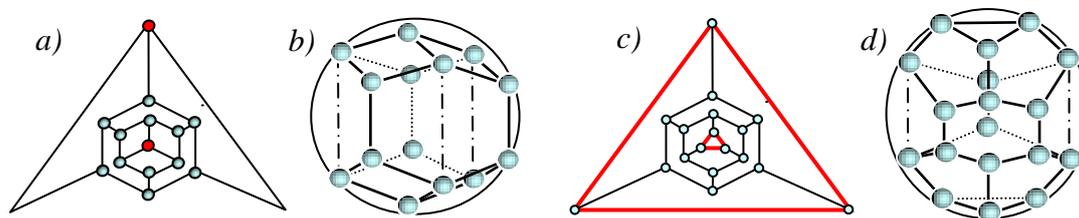


Fig. 13. Bi-shamrock: its graph (a) and atomic structure (b); and truncated bi-shamrock: its graph (c), and its atomic structure (d).

8. Conclusion

We have considered graphs describing the process of forming mini-fullerenes of small carbon clusters. On the basis of these graphs one can distinguish different families of mini-fullerenes and therefore one can make a classification of these unusual carbon structures.

Besides, we have done some innovation to the graph theory. We suggested considering a cluster of three or four atoms as a big point (vertex) contrary to a zero-size point (vertex) of a common graph. In this case we obtain a graph, which is identical to a simpler graph. It allows do some operations with this graph in same manner as with a usual graph that simplifies an analysis.

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