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Fusion reactions of cupola half fullerenes

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Abstract

Reactions of cupola half fullerenes C_{10}, C_{12}, C_{16}, C_{20} and C_{24} with each other are considered on the basis of Arrhenius's postulate. It means that at first there forms an intermediate compound and only afterwards a usual chemical reaction is going on. We supposed that during the reactions new covalent bonds are formed and some old covalent bonds between the reacting atoms are destroyed. The final structure of a fullerene is obtained through the use of geometric modeling. As applied to fullerenes, geometric modeling supposes that a forming fullerene tends to take the appearance of a perfect spheroid with equal covalent bonds. The graphs describing the process are constructed.

Keywords: Cupola half fullerene; Fusion reaction; Graph; Modeling.

1. Introduction

Up to now the fullerene-formation mechanism has remained a controversial point. Research suggests that fullerene assemblage originates of individual atoms and C_2-dimers, and, probably, of very small clusters. In Refs. [1,2] we have exhaustively investigated a dimer mechanism of fullerene growing. According to it, a carbon dimer embeds either into a hexagon or a pentagon of an initial fullerene. This leads to stretching and breaking the covalent bonds which are parallel to arising tensile forces. In both cases there arises a new atomic configuration and there is a mass increase of two carbon atoms. However, the above-stated mechanisms of fullerene growth are not unique. Fullerenes can be imagined to grow by reacting with each other, similar to a bubble growth in the soap solution.

This possibility was demonstrated by the example of such reactions as

$$C24 + C4 \rightarrow C_{28},\ C_{30} + C_6 \rightarrow C_{36},$$

and

$$C_{30} + C_{30} \rightarrow C_{60},$$

through the use of a new molecular dynamics that takes into consideration both atomic and electronic degrees of freedom simultaneously, especially the excited electronic states created by electronic transitions [3–6]. Fullerenes and nanotubes are formed at high temperatures and the new molecular dynamics, termed 'charged-bond' molecular dynamics, accounts for this factor properly. At first this molecular dynamics was developed as a rather sophisticated design, but later it obtained a strict theoretical basis [7].

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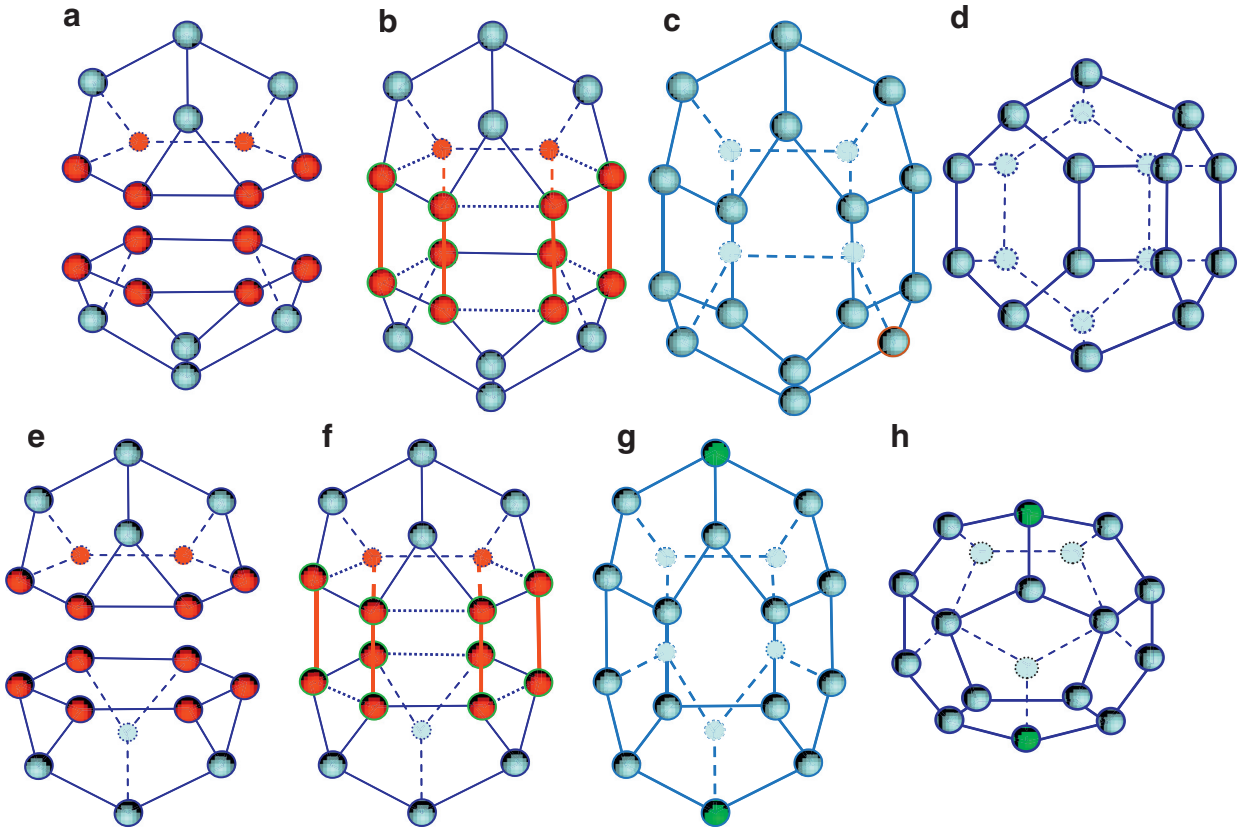

Fig. 1. Joining of two half-fullerenes C_{10} with the mirror symmetry (a–d) and the rotation-reflection symmetry (e–h): (a, e) Separate carbon cupolas C_{10}; (b, f) Intermediate compound; (c, g) Distorted polyhedron formed; (d) (Tetra-hexa)$_3$-penta$_6$ polyhedron C_{20}; (h) Dodecahedron C_{20} after relaxation; Red and blue spheres are reacting and neutral atoms, respectively; blue solid lines are covalent bonds; blue dashed lines are old covalent bonds to be destroyed; red solid lines are new covalent bonds. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Any molecular dynamics needs input data. For mini-fullerenes (up to C_{20}) the number of possible configurations is not very large, but as one passes to midi-fullerenes (C_{20}–C_{60}) one obtains a monstrous size 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. In this respect, it makes sense to use geometric modeling as a first step of a computer simulation and further theoretical analysis [8]. We suppose that the geometric modeling will allow us to envision a possible way of growing carbon clusters from the very beginning and thereby to decrease the number of configurations being worthy of further study.

In this contribution, we treat the growth of fullerenes as a series of joining reactions of cupola half-fullerenes C_{10}, C_{12}, C_{16}, C_{20}, and C_{24} [9] through the use of the geometrical modeling.

2. Reaction between two base-truncated triangular pyramids

The atomic configurations corresponding to reaction

$$C_{10}+C_{10}\rightarrow(C_{10}\ C_{10})\rightarrow C_{20}$$

between two base-truncated triangular pyramids C_{10} are presented in Fig. 1. At first two molecules C_{10} are moving towards each other (Fig. 1a). Then the atoms, marked in black, interact with each other producing a compound (Fig. 1b). New covalent bonds (heavy-black solid lines) have formed in this process, whereas the old covalent bonds between the reacting atoms (light-grey dashed lines) have splitted. As a result, a distorted polyhedron has formed (Fig. 1c), then it relaxes into a perfect polyhedron (Fig. 1d). The surface of its atomic configuration consists of three squares, three