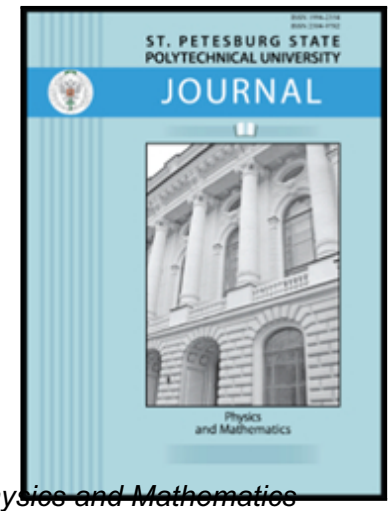

Geometric modeling of midi-fullerene growth from C_{32} to C_{60}

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Axonometric projections together with the corresponding graphs for fullerenes are constructed in the range from 32 to 60. The growth of fullerenes is studied on the basis of a 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 a hexagon adjoining two pentagons, two adjacent pentagons adjoining two hexagons are obtained. As a result, there arises a new atomic configuration and there is mass increase of two carbon atoms. We considered the direct descendants of fullerene C32; namely, C2n, where n = 17–30.

Fullerene; Modeling; Growth; Carbon dimer; Graph; Structure.

Introduction

Since the discovery of fullerenes [1, 2] and carbon nanotubes [3], carbon occupies a strategic position in materials science and technology as one of the most versatile and far-reaching materials [4, 5]. Obtaining fullerenes smaller than C_{60}, e.g., C_{36} [6] and C_{20} [7], has attracted considerable attention, since smaller fullerenes 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.

Current studies on fullerenes and their compounds mainly focus on large-size fullerenes. Experimental researches and practical applications of small-size fullerenes are still limited by their low yield and poor stability. The comprehensive experimental study on small or medium-size fullerenes revealed the following [8]. 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 $C_{49}H_{10}$. (We preserve here the terminology employed by the authors). However the structures of these molecules are not known; therefore theoretical methods are helpful in this field to identify some potential compounds with good properties.