

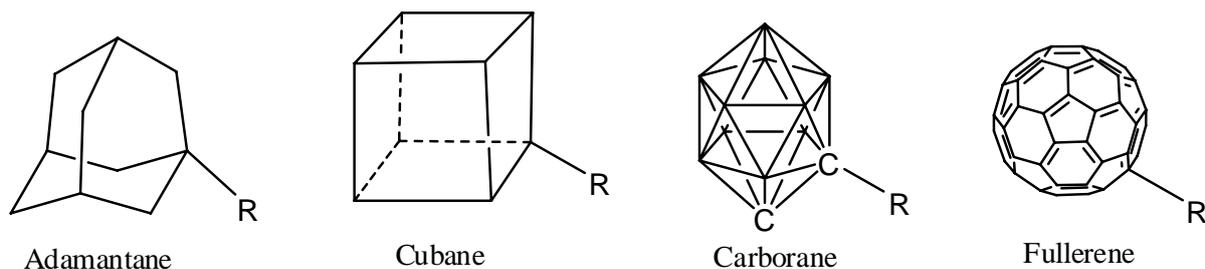
THE ADAMANTANE AND CARBORANE ANALOGS OF FULLERENE NANOCCLUSERS

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R – fragments of the molecule of carbohydrates, peptides, alkaloids, steroid hormones, lipids, and other bioactive compounds.

Introduction

Adamantane, *o*-, *m*- and *p*-carborane and fullerene nanoclusters and their derivatives find wide application in microelectronics, in the production of composite materials, in obtaining of nanomaterial for the needs of contemporary nanotechnology and in medicine [1-3].

At present the world-wide development of the new technology of the radiation therapy of tumor diseases – the neutron-trapping therapy of tumors. This technology is developed for the selective action on the tumor and it is the binary technology, which uses the tropic to the tumor preparations, containing the nuclides (^{10}B or ^{157}Gd , etc.), which, absorbing neutrons, form secondary radiation, disastrous for the tumor cells. In contrast to the traditional radiation therapy, the guidance to the target is carried out, first of all, by the selective concentration of preparations in the tumor, but not by aiming neutron beam. The irradiation of the struck cloths or organs serves as a basis for this technology and this technology eliminates the possibility of beam complications, since the dose of neutron emission does not exceed the tolerance of normal cloths, but the cumulative dose of radiation load on the malignant tumor is sufficient for its reliable therapeutic damage. For realization of the technology of the neutron-trapping therapy of tumor diseases there is a need to perform the search for the boron-containing preparations, enriched by the ^{10}B nuclide or the gadolinium-containing preparations with the ^{157}Gd nuclide, which must selectively be accumulated in the tumors in the concentrations of

more than 20 $\mu\text{g/g}$ of tumor for ^{10}B or 5.5 mg/g for ^{157}Gd [4,5].

The use of nanoclusters on the basis of adamantane, cubane, carboranes, fullerenes and other analogous compounds can serve as one of the promising trends of the search for the ways of selective delivery boron-, gadolinium- or other elementoorganic compounds into the struck cloths and the organs.

Results and the discussion

By the method of computer simulations with the application of methods of molecular mechanics and quantum-chemical calculations (semi-empirical model hamiltonian MNDO-PM3 and nonempirical calculations with using level HF/6-31G(d) and MP2/6-31G(d)), the effective volumes of the internal Van der Waals cavities of the derivatives of adamantane, *o*-, *m*- and *p*-carboranes and fullerenes C_{60-540} have been calculated. It has been established that the nanoclusters of adamantane, cubane and some other analogous skeleton connections can serve as "containers" for storage and transport of light ions H^+ , Li^+ , whereas the internal cavities of nanoclusters of carboranes and fullerenes are capable of containing both the atoms and molecules of a number of chemical elements and some connections [6,7].

The fundamental possibility and conditions both for the introduction and the emission of the atoms of inert gases, some metals, hydrogen and molecules of chemical compounds into Van der Waals' cavity of large nanoclusters has been investigated. The

possibility of application for these purposes of ultrahigh pressures, microwave emission, electron collision, quantum tunneling and inversion of external and internal surfaces of large nanoclusters has been studied. The lines of approaches to the chemical "building" of not completely formed large nanoclusters, after placement in their Van der Waals' cavity of the conjunctions, including method of constructing concentric fullerene nanoclusters, which contain 2 or the more inserted in each other structures have been directed. The possibility of production of carbonic graphite-like nanoclusters in the form of the Mobius tapes and Klein surfaces has been examined and the smallest possible sizes of these superchemical connections [8] have been calculated.

The methods of the synthesis of a number of the derivatives of adamantane, cubane, carboranes, fullerenes and another nanoclusters, which contain in their composition ester, acetylene, aromatic, peroxide, azomethine and other organic groups – convenient for the chemical immobilization have been developed. The chemical covalent additive products of nanoclusters with the natural amino acids, the peptides, terpenic and steroid alcohols, aldehydes and ketones, alkaloids, lipids and carbohydrates [9-21] have been formed and investigated.

Conclusions

The new aspects of the application of derived nanoclusters and compounds on their basis in biology and medicine, including in diagnostics and treatment of tumor diseases with the use of a binary radionuclide therapy have been studied.

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