Multifunctional silsesquioxanes as reactive building blocks for the synthesis of advanced molecular and macromolecular hybrid compounds

Research project objectives

The main aim of the project is the development of the methods for the synthesis of new alkenyl-functionalized silsesquioxanes *via* hydrosilylation reaction of the carbon-carbon triple bonds (C≡C), and further modification of obtained compounds by the palladium coupling reactions.

Silsesquioxanes are examples of well-defined, nanostructured, organic-inorganic compounds which have found wide applications in many areas of academic and industrial studies. Their easy functionalization *via* many catalytic processes (hydrosilylation, silylative coupling, cross-metathesis etc.) make them more and more attractive for researches what results in the increase number of scientific and patent publications (4740 publications, 27392 patents, according to Scopus 29.11.2017).

Part of these wide studies concerns alkenyl-functionalized silsesquioxanes. Up to date, they have been used in the synthesis of biomaterials, liquid crystals, fuel cells as well as solution processable organic (OLED) or polymer electronics (PLED). It has been established that the attachment of silsesquioxane as pendant groups onto conjugated molecules or polymers provides materials with improved color stabilities, higher brightnesses, and improved quantum efficiencies, compared with parent molecules or polymers that do not bear silsesquioxane groups. Moreover, such systems possess very good solubility in common organic solvents and improved mechanical, thermal properties. Not without significance is the fact that silicon-oxygen based core is biocompatible and non-toxic what with appropriate selection of alkenyl fragment makes resulted compounds useful for the medicine and pharmacy.

All of that makes that the synthesis of their new representatives is highly desirable.

Research within project

Within the project it is planned to design effective and selective methods for the synthesis of new alkenyl-functionalized silsesquioxanes with different, reactive functional groups, which will allow for their further modification *via* Heck, Suzuki and Sonogashira couplings.

The processes of the synthesis of the alkenyl-functionalized silsesquioxanes will be carried out *via* hydrosilylation reaction of symmetrically and non-symmetrically disubstituted alkynes and 1,4-disubstituted 1,3-butadiynes with mono- ($(HSiMe_2O)R_7Si_8O_{12}$) and tri(dimethylhydridosiloxy)silsesquioxane ($(HSiMe_2O)_3R_7Si_7O_9$) (where R= *i*-Bu, *i*-Oct, Ph) as well as octahydridospherosilicate ($(HSiMe_2O)_8Si_8O_{12}$). In the next step the modification of the selected compounds by Pd-catalyzed couplings will be performed.

The obtained compounds will be unique, multifunctional building blocks, characterized by interesting physio-chemical properties, which will find the application in the preparation of molecular and macromolecular hybrid systems.

Justification of the research

Due to the lack or scarce information about the synthesis of unsaturated silsesquioxanes *via* hydrosilylation reaction as well as process optimization and further modification of obtained molecules, it is highly justified to undertake research topics aimed at the synthesis and modification of these compounds.

Obtaining of the new multifunctionalized silsesquioxane derivatives, in a simple, highly efficient and selective way will be a breakthrough in the silsesquioxane chemistry, and thus will be crucial for the designing and synthesis of new materials with their uses.

Application of such wide spectrum of functionalized reagents with different structures, chemical, and physical properties will allow for comprehensive examination of the hydrosilylation process of the C≡C bonds, optimize its conditions and identify factors having the influence for its course.

The project fits in the ambitious challenges of synthesis (highly efficient and selective synthesis functional precursors for the synthesis of new materials) and is expected to contribute to the knowledge of the reactivity of C-C triple bonds in the hydrosilylation reaction.