

Silsesquioxanes, heterosilsesquioxanes, and borophosphates are macromolecular cage compounds with hybrid properties, i.e. combining both the features of inorganic and organic compounds. Owing to their unique properties resulting from their structure and elemental composition, these compounds are of considerable interest to a wide range of sciences such as synthetic and material chemistry, as well as engineering and physics of special materials.

Mechanochemistry is a subdivision of chemicals sciences that deals with phenomena caused by mechanical energy (grinding, pulverization, kneading). Mechanochemical phenomena had been already known in Antiquity, while their embedment on the ground of natural sciences took place at the turn of the nineteenth and twentieth century. Now, mechanochemical synthesis is increasingly gaining recognition in inorganic, organic and organometallic chemistry due to its simplicity, high efficiency and selectivity, straightforward scalability and "green chemistry" philosophy. The characteristic feature of mechanochemical synthesis is lack of solvent (or the addition of only small amount of liquid) during reaction, which significantly reduces the amount of produced waste products and ensures the peak concentration of reagents and maximum interactions between them. In most cases, the mechanochemical synthesis is carried out in devices called the ball mills, which possess special reaction vessels called grinding vessels (or jars), equipped with grinding balls. Ball mills put grinding jars into vibrations (the nature of vibrations depends on the type of device), which causes intensive contact of milling balls and high energy impacts with milled material, leading to its particle size reduction.

This project aims to utilize the mechanochemistry in the synthesis and functionalization (i.e. further expansion) of cage silsesquioxanes, heterosilsesquioxanes and borophosphates. The research carried out in the project aims to propose a simple and efficient alternative to standard reactions involving large quantities of solvents and reactive corrosive substances.

In short, the research proposed in the project is intended to lead to the application of mechanochemical transformations in the construction and expansion of cage compounds. This is to be achieved by using both partially condensed cage elements as well as by using basic building blocks, which are essentially simple compounds of the p-block elements. Symbolically, the idea of the project can be depicted as the formation of the Rubik's cube from large and small elements, as shown in the picture below.

