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VABILO NA PREDAVANJE V OKVIRU DOKTORSKEGA ŠTUDIJA KEMIJSKE ZNANOSTI / INVITATION TO THE LECTURE WITHIN DOCTORAL PROGRAMME IN CHEMICAL SCIENCES

Prof. dr. Pavel Matějíček

Department of Physical and Macromolecular Chemistry, Charles University, Faculty of Science, Czech Republic

z naslovom / title: Boron Cluster Compounds as Building Blocks in Nanochemistry

v sredo, 20. 10. 2021 ob 15. uri / on Wednesday, 20. 10. 2021 at 15.00,

v predavalnici 1 v 1. nadstropju Fakultete za kemijo in kemijsko tehnologijo, Večna pot 113 / *in lecture room 1, 1st floor at the Faculty of Chemistry and Chemical Technology, Večna pot 113*

Vljudno vabljeni! / Kindly invited!

Abstract:

Boron is one of the few elements that form large molecules through a series of covalent bonds. It yields borohydrides - boron cluster compounds, such as boranes, carboranes and metallacarboranes. The shape of boron clusters is atypical due to their electronic structure. The size of anionic boron clusters is within nano- and subnano-range, which differentiates them from classical inorganic anions. Besides 3D σ -aromaticity, they are characterized by negative partial charge of hydrogen atoms that has important consequences for their bonding, hydration and solution behavior. During the last decade, we have been extensively studying solution behavior of cobalt bis(dicarbollide) anion, COSAN, its derivatives and other anionic boron cluster compounds such as decaborate and dodecaborate dianions. The primary question stands what is a driving force of their self-assembly in water. Another important aspect is their interaction with co-solutes and macromolecules, and their distribution in micro-phases. Especially, the interaction of metallacarboranes with neutral hydrophilic polymers is almost unparalleled and it leads to unique hybrid nanostructures. To answer our questions, we employed synergistic combination of experiment, advanced computer simulations and quantum chemistry calculations. It is clearly evident that behavior of nanometer-sized anionic boron clusters cannot be described by paradigms and terminology established for classical ions, and such ions can be taken as unique building blocks in nanochemistry.