**Theoretical investigation of alkaline and alkaline-earth metals complexation with dibenzocrown ethers in fluorinated diluents**

***Ostras A.S.1, Timoshenko V.V.2***

*2nd Year PhD Student*

*1Infochemistry Scientific Center, ITMO University, 191002 St. Petersburg, Russia*

*2St. Petersburg State University, St. Petersburg, 199034 Russia*

*E-mail: [ostras@infochemistry.ru](mailto:ostras@infochemistry.ru)*

Crown ethers are extensive class of macrocyclic compounds, which for a long time widely used in different spheres of chemical sciences, like chemical analysis, chromatography, radiochemistry, construction of ion-selective electrodes and organic synthesis. Due to presence of certain size inner cavity in structure, crown ethers have unique ability to form strong complexes with various alkali and alkaline-earth metals in different media, which commonly used for metals separation.

Especially complexation properties of crown ethers towards alkali and alkaline-earth metals have great importance for development of new separation techniques of radionuclides from high-level waste (HLW), mainly radiocesium 137Cs and radiostrontium 90Sr, that can easily accumulate in water resources and therefore provide high damage on humans’ health and environment.

In this work we performed a quantum chemical modelling to study the complexation of different dibenzocrown ethers with different alkali and alkaline-earth metals in organic media. As complexing agents we considered 4,4’(5’)-di-tert-butyl-dibenzo-18-crown-6 and dibenzo-21-crown-7 ethers and as both organic diluents and media, we considered bis-(2,2,3,3-tetrafluoropropyl)carbonate (BK-1), bis(2,2,3,3-tetrafluoropropoxy)methane (FN-1) and 1-fluorooctane (FO-1); also, as media, we considered water. All calculations were carried out on density functional theory (DFT) level, which is a reliable and efficient electronic structure method for the supramolecular systems.

Our first main goal was to obtain the most possible structures of alkali and alkaline-earth complexes with crown ethers in water and organic solutions and evaluate their geometrical and electronic parameters. The second main goal was to study the thermodynamics of complexation process by determining stability constants of metal-crown complexes in different solutions.

