

In recent years one can observe a significant growth in research interest for the preparation of transition metal coordination compounds of high nuclearity. The properties of these new systems led to the development of novel functional molecular materials, photo-electronic devices and biomedical imaging probes and electron carriers in biochemical systems. One of the interesting classes of compounds bearing in their structure increased number of transition metal ions are metallocrowns (MCs). MCs are self-assembled, cyclic metal/organic compounds which are considered as crown ether analogues in their structure and function. The traditional definition of a MCs is a repeat unit of $-[M-N-O]_n-$ in a cyclic arrangement where the ring metal and nitrogen atom replace the methylene carbon atoms of a crown ether. As crown ethers they are characterized by the presence of a core cavity which may encapsulate a guest species.

Despite the fact, that slightly more than twenty years after their first characterization, the number of metallocrowns and related host-guest adducts isolated in the solid state grows every year numerous aspects which regulate their stability in solution and the correlation between the species isolated in solid state and those present in solution still remain insufficiently explored. More detailed characterization of the thermodynamic parameters and spectroscopic properties of MCs will be tremendously valuable and useful. Efficient adjustment of these parameters by appropriate choice of metal coordinating moieties and ligand dimensions is of particular importance in terms of MCs potential application as biomedical materials such as contrast agents, selective chelators of metals, or fluorescent probes.

The main objective of current project is to develop a series of hydroxamate ligands that will provide (i) a strong association with metal ions and a high thermodynamic stability of binary and ternary MCs in a broad range of pH, (ii) stability in the presence of bioligands, and (iii) ability to interact with bioligands. The first step to achieve this goal is to design and to examine the thermodynamic parameters of binary and ternary MCs. The finding of complexes stable in solution will allow us to move on to the investigation of the interaction of MCs with biologically important ligands, such as albumin or transferrin. By using our understanding of coordination preferences of metal ions and hydroxamate ligands and our previous achievements in the design of efficient metal chelators we would like to create a collection of MCs which exhibit the ability to interact with bioligands and stay stable in the presence of them.

To achieve the main goal, various physicochemical methods will be used. Combination of a variety of both common and sophisticated techniques will allow us to fully evaluate the physicochemical and thermodynamical characteristic of ligands and binary and ternary MCs.

We expect that the project will make a strong contribution to the overall knowledge in the field of coordination and solution chemistry of studied systems and will also emerge the best candidates for effective interaction with biologically important ligands.