

Thesis topics of the Department of Physical Chemistry, 2021/22/1.

Bényei Attila:

Use of crystallographic database (Chemist/Chemical Engineer MSc or BSc, 1 person, 1 free place)

Comparison of several structures determined by single crystal X-ray diffraction by using the Cambridge Structural Database. Analysis and comparison of secondary interactions and metal coordination in case of transition metal complexes. Learning the use of crystallographic software packages.

Novák Levente:

Formation of amide bond by thermal reaction in polar aprotic medium (MSc thesis, 1 person)

The amide bond formed by condensation between carboxyl and amino groups is of great importance for the synthesis of organic macromolecules owing to its hydrolytic stability and polar nature. In protic solvents (thus in water) it can only be formed indirectly from the appropriate amine and carboxylic acid due to the dissociation of these precursors. It is less known however, that in aprotic solvents amides can also form directly by thermal condensation. The reaction is probably made possible by the changed acid-base conditions, while the reaction equilibrium is shifted to the direction of the formation by the water solvation capacity of the solvent. We plan to investigate the kinetics of the reaction with small molecules, as well as with polymers, with special emphasis given to the acid-base conditions existing in the aprotic solvent.

Synthesis and characterization of functionalized macromolecules (MSc thesis, 1 person)

The properties of macromolecules are strongly influenced besides their chemical composition by other factors, as e.g. the structure of the carbon chain, the molecular weight and weight distribution of the polymer, spatial position of certain functional groups and their mutual distance. Macromolecules functionalized by suitable groups can be excellent ligands for different metal ions and the complexes so formed possess several advantages over the complexes of small molecules (decreased diffusion rate, easy separability, specific selectivity, kinetic stability). The synthesis of these macromolecules with specific properties is performed partly by linking together monomeric units, partly by the modification of existing polymers (called platforms).

Purification of the product from the starting materials and the byproducts of the reaction is an important step. Following the synthesis and the purification we will investigate the main properties of the macromolecules formed and/or the behavior of their most suitable metal complexes for a given area of application (colloidal catalysis, environmental protection, magnetic contrast agents).

Purgel Mihály:

Structural study of natural compounds and biologically active molecules by quantum chemical methods. (Chemistry BSc, no free place)

We do Density Functional Theory calculations to study the reaction mechanism of a relevant reaction of biologically active molecules. We try to calibrate our system by a well-known reaction and based on that we perform new calculations.

Tircsó Gyula:

Design, synthesis and characterization of Smart Imaging Probes (SCAs) for Magnetic Resonance Imaging

Magnetic resonance imaging (MRI) is a non invasive diagnostic tool that has long been used to obtain anatomical and functional images. In recent years, the new field of molecular imaging has emerged which looks for information at the molecular level by visualizing the concentration and function of bioactive molecules (glucose, citrate etc. concentration) or physiological parameters (pH, pO₂, etc.). The project aims to develop new systems for the imaging pH by MRI relying on our recent results (using platforms obtained as a results of fine tuning of physicochemical parameters of the complex), as well as coordination chemical characterization of the resultant complexes (stability and inertness of the complexes, relaxation properties etc).