Thesis topics of the Department of Physical Chemistry, 2023/24/2.

Attila Bényei:

Use of crystallographic database in comparison of solid-state structures. (Chemical engineer BSc/MSc, 1 person, 1 free)
Comparison of solid state structures is very important in the comprehensive analysis of metal complexes or biologically active organic molecules. The Cambridge Structural Database contains over 1 Million published structures. The task is to identify similar structures of a given compound family from the CSD and analysing their conformation in the solid state, describe the secondary interactions in the lattice and find links to the physico-chemical properties.

Synthesis and determination of structure of polymorphic pharmaceutically active compounds using X-ray diffraction. (Chemist/chemical engineer BSc/MSc, 1 person, 1 free)
Polymorphic forms and co-crystals of APIs are important in discovery science and pharma industry. These materials will be synthetized and characterized mainly using powder and single crystal X-ray diffraction methods.

Continuous symmetry measure for the analysis of solid state structure of metal complexes and hydrogen bond networks (Chemist or chemical engineer MSc, 1 person, 1 free)
Symmetry is a very important concept in several fields of science and art. In case of supramolecular analysis of solid state structures determined by X-ray diffraction the symmetry is defined as transformation of coordinates on set of points, i.e. atomic coordinates. In real cases the symmetry is broken, match of the coordinates is not exactly fulfilled. On the basis of continuous symmetry measure comparison of symmetry of metal complexes and/or hydrogen bond patterns will be done.

Levente Novák:

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.

Oldamur Hollóczki:

Studying the effect of polymers on the transfer of drugs through the blood-brain barrier (1 student, filled)
It has been shown in recent studies that polymer pollutants in food sources may interfere with the function of the brain in general, and the blood-brain barrier in particular. The student will study through molecular modeling the transfer of an antibiotic drug through the blood brain barrier, and the changes thereof if polymers (nanoplastics or chains) are dissolved in this membrane.

Rare Earths Research Group:

Complexes of the lanthanide ions (Ln3+) have been utilized in medical applications due to their widespread magnetic, photophysical, and nuclear properties. Owing to their toxicity the Ln3+ ions are must chelated using multidentate ligands. Beside the traditional pendant arms, the picolinate metal binding moiety is explored more extensively nowadays. The proposed project therefore aims at the development and synthesis of a monopicolinate based chelator derived form the 2,2'-oxybis(ethylamine) diamine possessing three acetate pendant arms (OBE3APA). The research will focus on the synthesis of the ligand and characterization (stability, formation and dissociation kinetics) of their complexes formed with metal ions of biomedical relevance (Bi^{3+}, Gd^{3+}, Sc^{3+} etc.).

Csupász Tibor és Tircsó Gyula
Proton exchange as a possible enhance the relaxivity of complexes - Synthesis and characterisation of new complexes (Chemistry BSc, 1 person, not free)