

## **Thesis topics of the Department of Physical Chemistry**

### **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, 1 person, 0 free)

Polymorphic forms and co-crystals of APIs are important in discovery science and pharma industry. These materials will be synthesized and characterized mainly using powder and single crystal X-ray diffraction methods.

**Structure determination of transition metal complexes using X-ray diffraction.** Chemist/chemical engineer MSc, 1 person, 0 free)

These materials will be synthesized in various academic research group. The task is to determine their structure, use of diffractometer, analysing the structures. Powder and single crystal X-ray diffraction methods will be applied