

<b>General Information</b>			
<b>Course name</b>	ÚCHV/VMS1/03 Computing Methods in X-Ray Structure Analysis	<b>ECTS Credits</b>	2
		<b>Semester</b>	summer
<b>Aims</b>			
Crystal structure analysis of simple samples, tabular and graphical processing of the results.			
<b>Content</b>			
<p>Practical course of crystal structures solution for substances with the number of atoms less than 1000 since data processing to publishing structures: selection of the right space group and generate the necessary files for the structure solution (Wingx); search for the model of the structure (SHELXS97, SIR97 and SUPERFLIP), refinement of the model (SHELXL97); graphical representation of the structure (DIAMOND); drawing of the structural scheme (ISIS DRAW); calculations of bond lengths, angles and hydrogen bonds (PARST); tabulation of the results of crystal structure analysis, obtaining the necessary data for similar structures from the Cambridge Structural Database System:</p> <p>Processing of results of powder diffraction technique, modeling of powder diffraction patterns (MERCURY).</p>			
<b>Assessment Methods and Criteria</b>			
Semester project.			
<b>Grading Scale (in %):</b> 100-91%-A, 90-81%-B, 80-71%-C, 70-61%-D, 60-51%-E, 50-0%-FX			

**Grading System:**

The University recognises the following six degrees for the evaluation of the study results:

- a) A – excellent (excellent results) (numerical value 1)
- b) B – very good (above average results) (1.5)
- c) C – good (average results) (2)
- d) D – satisfactory (acceptable results) (2.5)
- e) E – sufficient (results meet the minimum criteria) (3)
- f) FX – failed (requires further work) (4)

**Bibliography**

Manuals for the programs.

