

# Workshop program

## Monday 21 October

- 09:00 Opening (Michal Dušek)
- 09:10 Lecture: Restraints, constrains, rigid body (Michal Dušek)
- 09:30 Introduction to Examples (Michal Dušek)
- 09:50 Distribution of flash disks + installation of programs
- 10:00 Coffee break
- 10:15 Example 8.2 (Dinitros - application of rigid body for disorder )  
Example 8.1 (Terbut - application of rigid body for disorder)  
Example 2.3.2, 2.3.3 (MagCag – rigid body in a powder structure)
- 12:30 Lunch
- 13:30 Lecture: Introduction to modulated structures (for those who did not participate in the 17<sup>th</sup> workshop); crenel functions (for all) - (Václav Petříček)
- 14:00 Example 5.3 ( $\text{Cr}_2\text{P}_2\text{O}_7$  - Incommensurately modulated structure with discontinuous functions)
- 15:00 Coffee break
- 15:15 Example 5.3 (continued)  
Example 6.1 (KSm – modulated structure solved from powder data)
- 18:00 End

## Tuesday 22 October

- 09:00 Lecture: Commensurate structures (Michal Dušek)
- 09:30 Introduction to Examples (Michal Dušek)
- 09:40 Example 7.2 ( $\text{CrPOcom}$  – Solution of the low temperature commensurate phase of  $\text{Cr}_2\text{P}_2\text{O}_7$ )
- 10:00 Coffee break
- 10:15 Example 7.2 (continued)  
Example 7.3 (PhenanTin - Commensurate and supercell description of a five-fold superstructure)
- 12:30 Lunch
- 13:15 **Workshop photo** in front of the building A
- 13:30 Lecture: Composite structures, Five-dimensional structures (Václav Petříček)
- 14:00 Example 5.5 (Melilite - Incommensurately modulated (3+2)-dimensional structure)
- 15:00 Coffee break
- 15:15 Example 11.1 (Bezcox – Composite structure)  
Example 2.5 (Multiphase structure from powder data)
- 18:00 End of workshop