

Workshop program

Wednesday 14 March 2018

- 09:00 Opening (Michal Dušek)
- 09:10 Lecture: Introduction to Jana2006 (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 1.1 (Zn - simple structure from single crystal data)
Example 3.1 (AD3 - pseudomerohedric twin)
Example 3.3 (CsLiSO₄ - pseudomerohedric 3-fold twin)
- 12:30 Lunch
- 13:30 Example 3.2 (PyNinit – handling twin overlaps)
- 15:00 Coffee break
- 15:15 Example 4.1 (PtCu - disorder described with split atomic positions)
Example 4.2 (NaNiFe – mixed sites)
- 18:00 End

Thursday 15 March 2018

- 09:00 Lecture: Introduction to modulated structures (Václav Petříček)
- 09:30 Introduction to Na₂CO₃ (Michal Dušek)
- 09:50 Example 5.2 (Na₂CO₃ – simple modulated structure from single crystal data)
- 10:00 Coffee break
- 10:15 Example 5.2 (continued)
- 11:15 Introduction to Cr₂P₂O₇ (Michal Dušek)
Example 5.3.1 (Cr₂P₂O₇ – Processing of the area detector data by Crysalis)
- 12:30 Lunch
- 13:15 **Workshop photo** in front of the building A
- 13:30 Example 5.3.2 (Cr₂P₂O₇ - Incommensurately modulated structure with discontinuous functions)
- 14:30 Lecture: Powder structures with Jana2006 (J. Rohlíček)
- 15:00 Coffee break
- 15:15 Example 2.1 (PbSO₄ - simple structure from powder data)
Example 2.2 (Y₂O₃ – powder data with strong asymmetry)
- 16:15 Introduction to Example 2.4 – rigid body (Michal Dušek)
Example 2.4 (PFPhenyl – organometallic structure from powder data)
- 18:00 End

Friday 16 March 2018

- 09:00 Lecture: Commensurate structures (Michal Dušek)
- 09:30 Example 7.2 (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)
- 12:00 Lunch
- 13:00 Lecture: Five-dimensional structures (Václav Petříček)
- 13:30 Example 5.5.1 (Melilite – Processing of the area detector data in case of two q-vectors with overlaps)
Example 5.5.2 (Melilite - Incommensurately modulated (3+2)-dimensional structure)
- 16:15 Example 7.1 (Ephedrine - commensurately modulated structure with merohedric twinning)
- 17:15 Example 5.6 (Iodomol – application of rigid body for modulated molecule, manual data check for poor data)
- 18:00 End of workshop