Workshop program

Wednesday 19 April 2017

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 ($CsLiSO_4$ - 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)
18:00 End

Thursday 20 April 2017

09:00 Lecture: Introduction to modulated structures (Václav Petříček)
09:30 Introduction to Na_2CO_3 (Michal Dušek)
09:50 Example 5.2 (Na_2CO_3 – simple modulated structure from single crystal data)
10:00 Coffee break
10:15 Example 5.2 (continued)
11:15 Introduction to $Cr_2P_2O_7$ (Michal Dušek)
Example 5.3.1 ($Cr_2P_2O_7$ – Processing of the area detector data by Crysalis)
12:30 Lunch
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 ($PbSO_4$ - 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 21 April 2017

09:00 Lecture: Commensurate structures (Michal Dušek)
09:30 Example 7.2 (CrPOcom – Solution of the low temperature commensurate phase of $Cr_2P_2O_7$)
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)
14:30 Moving to building B (incl. computers)
Workshop photo in front of building A
14:50 (in building B)
Example 5.5.2 (Melilite - Incommensurately modulated (3+2)-dimensional structure)
16:10 Moving back to building A
16:15 Example 7.1 (Ephedrine - commensurately modulated structure with merohedric twinning)
17:15 Example 6.1. (KSm - modulated structure from powder data)
18:00 End of workshop