Workshop program

Time is given in UTC+1 (Prague)

Monday 7 December 2020

13:00 Opening (Michal Dušek)
13:10 Lecture: Introduction to Jana2020 and examples (Michal Dušek)
13:40 Download of documents, installation of Jana2020
Please use the latest Jana2020
14:00 Solution of examples
Participants will independently solve examples and contact lectors in case of troubles using Zoom
Example 1.1. Zn
Simple structure from X-ray single-crystal data
Example 2.1.1 $PbSO_4$
Simple inorganic structure from X-ray powder data
Example 3.1 AD3
Simple structure with pseudo-merohedric twinning
Example 4.1 PtCu
Disordered structure
17:00 End of workshop

Tuesday 8 December 2020

13:00 Lecture: Introduction to twinning options (Václav Petříček)
13:30 Step-by step introduction to Example 3.3.1 (Václav Petříček)
14:30 Solution of examples
Participants will independently solve examples and contact lectors in case of troubles using Zoom
Example 3.3.1 CsLiSO4
Simple structure with reticular pseudo-merohedric 3-fold twinning
Example 3.2 Pyninit
Simple structure with non-merohedric twinning. Handling twin overlaps
17:00 End of workshop

Monday 14 December 2020

13:00 Lecture: Introduction to modulated structures (Václav Petříček)
13:30 Step-by step introduction to Example 5.1 (Václav Petříček)
14:30 Solution of examples
Participants will independently solve examples and contact lectors in case of troubles using Zoom
Example 05.1 YPO
Simple structure where a light atom has a discontinuous modulation function.
Example 05.2 Na_2CO_3
Simple structure with strong harmonic modulation.
17:00 End of workshop

Tuesday 15 December 2020

13:00 Lecture: Introduction to powder structures (Jan Rohlíček)
13:30 Step-by step introduction to Example 2.4 (Jan Rohlíček)
14:30 Solution of examples
Participants will independently solve examples and contact lectors in case of troubles using Zoom
Example 02.4 PFPhenyl
Refinement of an organometallic structure from powder data with help of geometry constrains.
Example 02.7.1 $LaPO_4$
Crystallite size by fundamental approach.
17:00 End of workshop

Thursday 14 January 2021

13:00 Lecture: Collection of 3D ED data (Mariana Klementová)
13:45 Lecture: Data processing with PETS 2.0 (Lukáš Palatinus)
14:30 Installation of software (PETS, VESTA)
14:45 Solution of examples – data processing
Participants will independently solve examples and contact lectors in case of troubles using Zoom.
Example 13.1 Pyrite – very simple inorganic structure
Example 13.2 paracetamol
Example 13.3 borane - optional
17:00 End of workshop

Friday 15 January 2021

13:00 Lecture: Structure refinement of 3D ED data (Lukáš Palatinus)
14:00 Solution of examples – kinematical and dynamical structure refinement
Participants will independently solve examples and contact lectors in case of troubles using Zoom.
Example 13.1 Pyrite – very simple inorganic structure
Example 13.2 paracetamol
Example 13.3 borane - optional
17:00 End of workshop