

# Workshop program

**Time is given in UTC+1 (Prague)**

## Monday 8 March 2021

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 01.1. Zn

*Simple structure from X-ray single-crystal data*

Example 02.1.1 PbSO<sub>4</sub>

*Simple inorganic structure from X-ray powder data*

Example 04.1 PtCu

*Disordered structure*

17:00 End of workshop

## Tuesday 9 March 2021

13:00 Lecture: Introduction to twinning options (Václav Petříček)

13:30 Step-by step introduction to Example 03.3.1 (Václav Petříček)

14:30 Solution of examples

*Participants will independently solve examples and contact lectors in case of troubles using Zoom*

Example 03.1 AD3

*Simple structure with pseudo-merohedric twinning*

Example 03.3.1 CsLiSO<sub>4</sub>

*Simple structure with reticular pseudo-merohedric 3-fold twinning*

Example 03.2 Pyninit

*Simple structure with non-merohedric twinning. Handling twin overlaps*

17:00 End of workshop

## Wednesday 10 March 2021

13:00 Lecture: Introduction to modulated structures (Václav Petříček)

13:30 Step-by-step introduction to Example 05.1 (Václav Petříček)

14:30 Solution of examples

*Participants will independently solve examples and contact lectors in case of troubles using Zoom*

Example 05.2  $\text{Na}_2\text{CO}_3$

*Simple structure with strong harmonic modulation.*

Example 05.1 YPO

*Simple structure where a light atom has a discontinuous modulation function.*

17:00 End of workshop

## Thursday 11 March 2021

13:00 Lecture: Introduction to powder structures (Jan Rohlíček)

13:30 Step-by-step introduction to Example 02.4 (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  $\text{LaPO}_4$

*Crystallite size by fundamental approach.*

17:00 End of workshop