

Ab initio structure determination with powder diffraction data

Theory and hands-on short course

Program

Day 1

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 **Introductory crystallography:** unit cell, symmetry elements of macro- and microcrystallography, crystal structures, seven crystal systems, 14 Bravais lattices, space groups,

10:30 – 11:50 Coffee Break

11:50 – 13:00 **X-ray diffraction:** Miller indices, atomic scattering factors, anomalous dispersion; X-ray sources, choice of radiation, wavelength, resolution, mass absorption,

13:00 – 14:00 Lunch

14:00 – 15:30 **Data collection:** Data collection, reduction, aberration correction, preferred orientation

15:30 – 15:50 Coffee Break

15:50 – 17:00 **Powder data indexing:** manual and automatic indexing of powder data

Day 2

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 **Space groups:** Introduction to crystallographic space groups, alternative space groups, sub- and supergroups.

10:30 – 11:50 Coffee Break

11:50 – 13:00 **Space group assignment:** assignment of space groups

13:00 – 14:00 Lunch

14:00 – 15:30 **Extraction of structure factors:**

15:30 – 15:50 Coffee Break

15:50 – 17:00 *Phase problem:*

Day 3

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 *Phase problem, structure recycling, Fourier synthesis*

10:30 – 11:50 Coffee Break

11:50 – 13:00 *Rietveld refinement*

13:00 – 14:00 Lunch

14:00 – 15:30 **Practical session**

15:30 – 15:50 Coffee Break

15:50 – 17:00 **Practical session**

Day 4

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 **Practical session**

10:30 – 11:50 Coffee Break

11:50 – 13:00 **Practical session**

13:00 – 14:00 Lunch

14:00 – 15:30 **Practical session**

15:30 – 15:50 Coffee Break

15:50 – 17:00