

Course curriculum – ND/PUC Chemical Crystallography August 13 to August 18, 2018

Lectures will be held in the mornings, workshops in the late morning and afternoon.

Monday, August 13

Morning

Lecture: Introduction/Background (Oliver)

Lecture: Space groups/Symmetry/Diffraction (Sevov)

Afternoon

Workshop: SHELX – INS file and HKL file (Iluc)

Workshop: Software Familiarity/Solving Structures/Refining Structures (ShelxLE) (Iluc/Oliver/Sevov)

Tuesday, August 14

Morning

Lecture: Structure Factors/Structure Refinement (Sevov)

Lecture: Structure Solution Techniques - Patterson Methods, Direct Methods, Charge Flipping, Intrinsic Phasing (Oliver)

Afternoon

Workshop: Structure Solution/Structure Refinement (OLEX2) (Iluc/Oliver/Sevov)

Wednesday, August 15

No class: National Holiday

Thursday, August 16

Morning

Lecture: Structure Validation/Finalization (Oliver)

Lecture: Crystallographic Databases (Iluc)

Afternoon

Workshop: Disorder and problem structures (Iluc/Oliver/Sevov)

Friday, August 17

Morning

Lecture: Powder Diffraction (Oliver)

Workshop: PLATON (overview) (Iluc)

Afternoon

Workshop: Structure finalization and report generation (Iluc/Oliver/Sevov)

Saturday, August 18

Morning

Certificate presentation / Discussion