Course curriculum – ND/PUC Chemical Crystallography August 13 to August 18, 2016

Lectures will be held in the mornings, workshops in the afternoon.

Monday, August 13

Lecture: Introduction/Background (Oliver)

Lecture: Basic concepts of crystallography (Oliver)

Lecture: Space groups/Symmetry (Sevov)

Workshop (afternoon, Tue Aug 16): SHELX – INS file and HKL file (Iluc)

Workshop (afternoon, Tue Aug 16): Software Familiarity/Solving Structures/Refining Structures (ShelxLE) (Iluc/Oliver/Sevov)

Tuesday, August 14

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

Lecture: Structure Refinement: Least squares (Sevov)

Workshop: (afternoon, Wed Aug 17) Structure Solution/Structure Refinement (OLEX2) (Iluc/Oliver/Sevov)

Wednesday, August 15

Holiday: Assumption of Mary

Thursday, August 16

Lecture: Structure Validation/Finalization (Oliver)

Lecture: Crystallographic Databases (Iluc)

Workshop (afternoon Thu Aug 18): Disorder and problem structures (Iluc/Oliver/Sevov)

Friday, August 17

Lecture: Powder Diffraction (Oliver)

Lecture: Standard uncertainties (Sevov)

Workshop (afternoon, Fri Aug 19): PLATON (overview) (Iluc)

Workshop (afternoon, Fri Aug 19): Structure finalization and report generation (Iluc/Oliver/Sevov)

Saturday, August 18

Software use and certificate presentation.