

Summer School on Polycrystalline Structure Determination

The School Director: Prof. C. Giacovazzo, *Italy*

Thursday - 24 September

20.00 - *Well-together-party*

Friday – 25 September

8.25 - 8.30 – School presentation;

8.30 - 10.00- Peak search, indexing, space group determination (*Carmelo Giacovazzo*)

10.00 - 11.30- Using multiple datasets to get a better estimation of structure factor amplitudes:
anisotropic thermal expansion and texture effects (*Lynne Mc Cusker*)

11.30 - 12.00 – *Coffee break*

12.00 - 13.00 - Direct Methods (*Carmelo Giacovazzo*)

13.00 - *Lunch*

15.00 -17.00 - Direct space approaches for phasing powder data

15.00-15.30- Applications of parallel tempering by FOX (*Wieslaw Lasocha*)

15.30- 16.00 - Simulated annealing in EXPO2009 (*Carmelo Giacovazzo*)

16.30- 17.00 – POLPO in EXPO2009 (*Carmelo Giacovazzo*)

17.00 – 17.30 – *Coffee break*

17.30-19.30 Computer session (Indexing and space group determination by EXPO2009 (*Corrado Cuocci*);

20.00 - *Folkloristic Dinner*

Saturday – 26 September

9.00 - 10.30 - Rietveld Refinement (*Wieslaw Lasocha*)

10.30 - 11.30 - Solving zeolite framework structures from powder diffraction data (*Lynne Mc Cusker*)

11.30 – 12.00 - Coffee break

12.00 - 13.00 - Rotation camera and 3d diffraction tomography . Phasing from powder nanocrystals (*Stavros Nicolopoulos*)

15.00 - 16.00 Modulated and composite structures from powder diffraction (*Vaclav Petricek*)

16.00 – 16.30 – Coffee break

16.30 - 18.30 Computer session : solution of modulated structures Superflip / Jana 2006 (*Vaclav Petricek*)

19.30 - Dinner

Sunday – 27 September

9.00 - 11.00 – *Miscellanea* :

- a) Free time for student presentations;
- b) Restrainted Rietveld refinement: examples (*Wieslaw Lasocha*)
- c) Resolution bias correction and applications to Powders (*Carmelo Giacovazzo*)

11.00- 11.30- Coffee break

11.30-13.00- Computer session : Reciprocal and Direct Space Methods for Crystal structure solution in EXPO2009(*Corrado Cuocci*)

13.00 - Lunch