1st Excelsus Structural Solutions' Advanced Training 9-12 September 2015, Bologna, Italy



Advanced Training in X-Ray Crystallography with Carmelo Giacovazzo

Excelsus Structural Solutions in collaboration with the "G. Ciamician" Chemistry Dpt at the University of Bologna (Prof. Lucia Maini) organizes the 1st of a series of advanced trainings addressed to a <u>scientific industrial audience</u> with interest in X-Ray Powder Diffraction and its applications to <u>small organic molecular compounds</u>.

Topic of this 1st event is **X-Ray Crystallography** with lectures delivered by

Prof. Carmelo Giacovazzo

Consiglio Nazionale Ricerche,

Institute of Crystallography (CNR-IC)-Bari, Italy

When: **September 9th-12th** (intensive, all day)

Where: "G. Ciamician" Chemistry Department, University of Bologna - Italy



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Lectures topics:

General crystallography: Space group symmetry; the metric matrix; the reciprocal lattice; mathematical background: the concept of convolution and Fourier Transform; mathematical model of a lattice and of a crystal; Thomson–Compton scattering; interference of scattered waves; scattering from atomic electrons, atoms, molecules; isotropic and anisotropic temperature factor; crystal diffraction: the Laue condition; the structure factor; reflection and limiting spheres; symmetry in reciprocal space: Laue groups, symmetry restricted phase reflections, systematic absences, determination of the space groups; the calculation of the electron density; crystallographic Least Squares; Single Crystal and Powder Diffraction

Powder Crystallography: unit cell determination; space group determination; Full Pattern decomposition; LeBail and Pawley refinements, Direct- Patterson Methods; resolution Bias correction; direct space phasing techniques, simulated annealing, Rietveld refinements; XRPD Software Demos.



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Interested people should contact:

<u>Crystallography-Lectures@excels.us</u> OR <u>fabia.gozzo@excels.us</u>

(see also www.excels.us OR http://www.ciam.unibo.it/crystal_engineering)

- Limited number of participants, first-comes first served
- ➤ Registration fees: 800 Eur (before May 30th), 1200 Eur (after May 30th)
- Mandatory: study of the first 24 pages of Fundamentals of Crystallography (2nd Edition) plus exercises assigned by Carmelo Giacovazzo prior to the lectures! Material (i.e. 24-pages + exercises) distributed by Excelsus to the confirmed participants 3 months before the training!
- Any question about the distributed material? Carmelo Giacovazzo is available to answer them BEFORE the lectures via email.

What you should know about these lectures

- ☐ These are **interactive lectures**: you will learn X-Ray Crystallography step-by-step and check at each step with lots of exercises whether everything is clear.
- ☐ The atmosphere is friendly so that participants would never hesitate asking questions. The rhythm is advanced, but besides the mandatory first 24 pages of *Fundamentals of Crystallography* and introductory exercises, you are not expected to be already a skilled crystallographer.
- ☐ If you think crystallography is boring or difficult, you have never had the chance to attend lectures like these!