



PRESENTATION

PRESENTACIÓN

José Miguel Mancheño

Instituto de Química-Física Rocasolano
Consejo Superior de Investigaciones Científicas
xjosemi@iqfr.csic.es

Copyright: © 2015 CSIC. This is an open-access article distributed under the terms of the Creative Commons Attribution-Non Commercial (by-nc) Spain 3.0 License.

The year 2014 was declared the International Year of Crystallography (IYCr2014) by the United Nations to celebrate 100 years of this modern science, following the first Nobel prize related to crystallography, awarded to Max von Laue. During this year the International Union of Crystallography (IUCr), together with UNESCO, has organized many different activities worldwide thanks to the support from industrial and academic sponsors. The events have ranged from Science Fairs for schoolchildren, to professional-level Open-Lab workshops and training sessions, to international summit meetings to shape future policy. Additionally, the IUCr launched a new fully open-access journal (IUCrJ) and also prepared its journals (*Acta Crystallographica Sections A-F*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*) for the new developments in crystallography.

The main objective of the IYCr2014 has been to raise awareness about the importance of crystallography in the modern world perhaps motivated by the concern that crystallography lives in our society in a state of latency. Many different and complex reasons may explain this situation and one of them is probably related to the teaching of crystallography. As it has been recognized (Dauter & Jaskolski, 2010), crystallography is in this sense a peculiar science since it

is at the same time interdisciplinary (it overlaps with physics, chemistry and biology) and yet rather hermetic. Although traditionally it has been taught in the faculties of Physics, Chemistry or even Biology or Geology, currently the attention paid to crystallography in university curricula is waning, hence there is a real danger that next generation of scientists will not be properly formed in this discipline. The IYCr2014 has fought rigorously against this situation.

The IYCr2014 has witnessed the publication of excellent reviews on diverse aspects on the evolution that crystallography has experienced during the last 100 years, and probably one of the most meticulously analysed were the technological ones followed by historical analyses. Developments in crystallography are intimately associated to technological advances, mainly from the second half of the last century when the conceptual framework for biological crystallography was firmly established: at that moment, the knowledge was already there, what was lacking was the technology (Baker, 2014). Thus, the amazing expansion of crystallography during the last 50 years has been driven by technological advances like recombinant DNA technology, computing, synchrotrons, X-ray detectors, optimized crystallization methods, new algorithms for phasing and refinement and so on.

Still in the context of the IYCr2014, Arbor wanted to make its contribution in favour of crystallography by preparing a set of review articles covering the last 100 years of this science, mainly focusing of methodological aspects together with some historical ones. Thus, Celerino Abad-Zapatero discusses relevant events within biological crystallography from a personal perspective. Julia Sanz reviews the important and frequently overlooked roles that women have played in crystallography, and Guillermo Montoya takes us on a guided tour of Structural Biology through X-ray crystallography. The methodological articles start with that from Isabel Usón who reviews current methods for crystallographic structure solution, followed by

those from Pavel Afonine, Alexandre Urzhumtsev and Paul D. Adams, and Eugene Krissinel, who review macromolecular crystallographic structure refinement and the CCP4 software suite, respectively. The history, evolution and technology behind synchrotrons are summarized by Gavin Fox and finally, the article by Enrico A. Stura describes about protein crystallization methods for drug design.

In addition, with the aim to get insights into the future of crystallography, Arbor interviewed other relevant scientists namely Paul Adams, G. R. Desiraju, Kay Diederichs, Sine Larsen, and Martín Martínez-Ripoll from different fields of crystallography.