International Union of Crystallography (IUCr) Activities' Report - Year 2016

Delegate: Carlo Mealli (CNR-ICCOM)

1. Introduction

The IUCr has as target the promotion of the international cooperation in crystallography. The task is not straightforward, because crystallography is highly multi-disciplanary and operates in remote areas of science. The common goal is determining the relations between structure and properties in ordered materials, which span from proteins to drugs, technological species to minerals, including those of extraterrestrial origin. Since 1946, the IUCr promotes and coordinates researches of this type within the international scientific communities to favor a shared culture, the standardization of the methods, innovative collaborations even between very distal subjects, the construction and usage of large facilities, publications in journal of common crystallographic interest, the development of the crystallographic knowhow including less favored countries, the organization of schools and scientific events. In 2014, the International Year of Crystallography (IYCr2014), promoted by the ONU and carried out in strict collaboration with the UNESCO, has been a powerful vehicle for the educational activities of the crystallographic culture also in developing countries with the opening of new laboratories after proper training of the personnel. The thrust forward is continuing to be fruitful. Italy, in particular, has strategically contributed in the mentioned directions, because it participates since many years in the IUCr activities, often including management and governance.

2. Main activities carried on by (Union name) during 2016 relevant for Italy and for CNR

The IUCr holds its Congress and General Assembly every three years (the next XXIV IUCr Congress will be in August 2017 in Hyderabad, India). In 2016, the congress of interest for the Italian crystallographic community was that held in Basel (Switzerland), organized by the European Crystallographic Association (ECA), *i.e.*, a regional body of the IUCr. The president of ECA is now the Italian prof. Alessia Bacchi of the University of Parma. At the ECA Council, the Italian delegates were pleased to verify the large consensus given to the European Crystallographic School (ECS), first proposed by the Italy. The latter is now a sound and appreciated tradition, to be repeated every year in a different EU country. The first ECS in Pavia (2014) was extremely successful. The event continued in Croatia (2015) and Spain (2016), at it will be hosted by Poland in 2017.

The IUCr continues to support other numerous crystallographic events in Europe, one of the most prestigious ones being the international school of Erice (Sicily). The CNR, as the Italian "adhering body" of the IUCr, represents the basic reference of the Union's activities. For instance, the recent birth of the Albania's Crystallographic Association, interconnected with Associazione Italiana di Cristallografia (AIC) and with the scientific support of the Instituto di Cristallografia (CNR-IC).

3. Activities carried on by Carlo Mealli within the Union during 2016 and impact on the Italian scientific community

Mealli has been confirmed as the CNR delegate at the IUCr in the year 2015, with Michele Saviano (CNR-IC) being the substitute. At the end of 2015, Mealli was also confirmed member of the consulting commission for the participation of CNR to the IUCr (see the following point 7). With his involvement, he has stimulated discussions and initiatives for a proactive role of the CNR in the international scene. In the ECA, Mealli is the chair of the General Interest Group of Senior Crystallographers (GIG2) and, for years, he is an auditor of the ECA budget. Thus, he regularly participates in the ECA Council and presents economic reports. Also, he has been one of the main

promoters of the ECA schools (ECS) for the education of young researchers. Analogously, he promoted joint crystallographic congresses of Italy and other European nations, such as the Italo-Spanish one (MISCA), which is held every three years. At its fourth edition in 2016 (Tenerife, Spain), Mealli was awarded the MISCA gold medal, established in recognition of important scientific contributions but also the activity for the diffusion of crystallography at the international level. For years, as member of a dedicated CNR commission, Mealli has monitored the relations between CNR and ICSU (International Council for Science), of which the IUCr is a major member. In particular, he has always recommended to CNR (especially as a member of the CNR Scientific Council (2012-2016)) an intense cooperation with ICSU. Presently, an Italian scientist, Dr. Lucilla Spini, is the head of the ICSU scientific programs, hence she can in principle provide precious information on projects to which Italian researchers can apply and contribute. For these reason, the contacts with Dr. Spini should be highly encouraged by the CNR. In this respect, it is worth mentioning that the application to the 'ICSU Grants Programme 2016-2019', made in collaboration between IUCr and IUPAP (International Union of Pure and Applied Physics), has been funded with €300000. In particular, the project "Utilisation of Light Source and Crystallographic Sciences to Facilitate the Enhancement of Knowledge and Improve the Economic and Social Conditions in Targeted Regions of the World" has been presented by the Italian researchers, Michele Zema (University of Pavia) for the IUCr and Sandro Scandolo (ICTP, Trieste) for IUPAP.

4. Evaluation of the participation in terms of benefits and membership cost

IUCr with more than 20000 followers is one of the largest scientific Unions in the world and it continues to grow thanks to new national bodies, whose interest emerged within the International Year of Crystallography (IYCr2014). For being multi-disciplinary, crystallography falls at the frontiers of different sciences and technologies, especially for addressing the structures of new materials and their applications. The fundamental character of crystallography is testified by the many Nobel prizes awarded to its subject experts in medicine, chemistry, physics (from the DNA characterization to that of ribosomes, superconductors, aperiodic crystals and more). Italy has a prominent role in the international crystallography for the historical value of its contributions but also its potentialities in the various fields. It is therefore highly desirable to remain in such an elite and especially for this the CNR should continue to pay the yearly fee of about 6000 euro for the membership. The cost does not seem excessive especially in view of the many benefits for both the national crystallographic community and the entire scientific interest of the nation.

5. Evaluation of Italians' attendance and how to improve interest and involvement

Mealli, as the CNR delegate to the IUCR, stays in continuous touch with the CNR-IUCr commission and the Italian Outreach officer of the Union, to favor a proactive participation of Italy in the IUCr activities and programs. The Italian community has at least one member in almost all of the scientific commissions, aimed to the prosperity of crystallography in each different area. These members supply continuous indications on the topics to be pursued and the events to be followed. Also the AIC, presently chaired by prof. Giuseppe Zanotti (UniPd), is in continuous contact with the IUCr, being often consulted about initiatives and strategies. Furthermore, the Italian colleague Dr Michele Zema (Unipv) has in the past years assumed very important roles in the governance of the IUCr, since he first served as the general manager di IYCr2014, having great success as organizer of the events and fund raiser. As stated, he become in 2016 the "Outreach Officer" of the Union with a central powerful role. In fact, by operating in symbiosis with the Executive Committee and the Editor-in-Chief, he ensures scientific continuity and new openings also to new branches of science, which use crystallographic techniques. Moreover, he coordinates: i) worldwide development activities and, in particular, in less favored countries; ii) initiatives for the IYCr Legacy (OpenLabs etc); iii) relations with UNESCO and other research institutions controlled by governments or other international scientific societies. As a result, Italy's participation in the IUCr has increased importance with continuous flow of information about emerging scientific themes, projects and programs, hence favoring new contacts between researchers and advantages for the CNR itself.

6. Italian experts with important roles within the Union or within related Commissions and Programs (if known)

Several Italian researchers have apical roles in the international crystallography. Besides (Alessia Bacchi) and the IUCr officer (Michele Zema), it is important to mention Andrea Zappettini (CNR-IMEM) as an ex-office member of the Executive Committee of the International Union of Crystal Growth (IUCG), of which Roberto Fornari (UniPr) is Past President. Also, Matteo Leoni (UniTn) is chair of the Board of Directors of the International Centre for Diffraction Data (ICDD). There are other 14 Italian members in the IUCr commissions and 3 chairs. The commissions do not only outline the frontier areas of research in their specific sectors, but are also fundamental in proposing the most reklevant speakers in the numerous international congresses. Below, the names of the involved Italian colleagues are presented in detail.

Chairs

Gilberto Artioli (UniPd and member of the CNR-IUCr commission) chairs the commission "Crystallography in Art and Cultural Heritage" since 2014; Piero Macchi (presently at the University of Bern) chairs the commission "Charge, Spin and Momentum Densities" since 2014); Andrea Zappettini (CNR-IMEM and member of the CNR-IUCr commission) chairs the commission "Crystal Growth and Characterization of Materials" since 2011.

Members

Angela Altomare (CNR-IC), Powder Diffraction (since 2014); Ross Angel (UniPd), High Pressure (since 2014); Giuliana Aquilanti (ELETTRA), XAS (since 2014); Federico Boscherini (UniBo and member of the CNR-IUCr commission), Crystallographic Nomenclature (since 2014) e International Tables ed Editor vol. I (since 2014); Andrea Cornia (UniBo), Magnetic Structures (since 2014); Roberta Oberti (CNR-IGG and president of the CNR-IUCr commission), Inorganic and Mineral Structures (since 2014); Silvia Onesti (ELETTRA), Biological Macromolecules (since 2011); Davide Proserpio (UniMi), Mathematical and Theoretical Crystallography (since 2008); Paolo Radaelli (affiliated in UK), Neutron scattering (since 2011); Giuseppe Resnati (UniMi), Structural Chemistry (since 2011); Davide Viterbo (UniPO), Crystallographic Nomenclature (since 2011); Michele Zema (UniPv and associate CNR-IGG), Crystallographic Teaching (since 2014).

7. If Union with CNR Commission, short summary about the 2016 CNR Commission activities

The Commission of the participation of CNR to IUCr has been renewed at the end of 2015. Its members, besides Carlo Mealli, are Gilberto Artioli, Federico Boscherini, Andrea Ilari, Roberta Oberti, Michele Saviano, Giuseppe Zanotti, Andrea Zappettini e Michele Zema. Oberti e Saviano have been elected as president and secretary of the commission. Since 2016 has been a year of preparation of the next XXIV IUCr congress and General Assembly in Hyderabad, India (2017), the Commission has worked (also through internet reunions) to present valid proposals to the organizing committee. A first goal has been that of supporting contributions to the congress from our crystallographic community. The result has been satisfactory, also because Italy has three members in the Congress International Program Committee (IPC) (Gilberto Artioli, Andrea Zappettini e Piero Macchi) plus one member in the Local Organizing Committee (Michele Zema, as observer of the IPC). In particular, one of the plenary speakers is the Italian Giacomo Chiari, who presently lives in the USA. Other keynote lectures are Dario Braga, Matteo Leoni, Massimo Nespolo, Sakura Pascarelli and Giuseppe Resnati, with Nespolo e Pascarelli living in France. There are also numerous chairs of microsimposia (Alessia Bacchi, Paolo Falcaro, Pierangelo Metrangolo, Mauro Gemmi, Giuliana Aquilanti, Nicola Casati, Isabella Pignatelli, Francesco Mezzadri, Roberto Mosca, Annalisa Guerri, Michele Zema).

The CNR commission has proposed two new Italian members for the IUCr commissions, namely Annalisa Guerri (UniFi) and Beatrice Vallone (UniRoma1 and associate researcher at CNR-IBPM). Finally, the Commission has named three Italian delegates to the next IUCr General Assembly CNR (Mealli, Zanotti and Zappettini).

8. Conclusions

As the CNR delegate at the IUCr, I wish to remark the great vitality of the Union as a first class scientific organization, whose mission is well illustrated in its website www.iucr.org. In Italy, the great majority of Italian crystallographers participates in its activities, but also in those of the European regional body ECA (European Crystallographic Associations) with many members and responsible persons from our country, as it may be verified in the website www.ecanews.org. I like to recall, that the AIC operates for involving some of its members at the international level and, in this respect, has presented many suggestions in the last years (check the website www.cristallografia.org). Therefore, there are multiple reasons to recommend to the CNR the continuation of the Italian participation in the IUCr, given that Italy is one of its most relevant members. Additionally, many Italian researchers deserve to be supported at the best by the national Institutions, especially when working for the promotion of international initiatives, such as for instance the organization of schools, congresses, workshops. Only in this manner, our community can attain a heavier weight in the crystallographic world and consequently in the wider science.

Honestly, Dr. Carlo Mealli (Professor of Research)

Carlo Heall!

Sesto Fiorentino, April 12th 2017