International Union of Crystallography, IUCr Activities' Report - Year 2018

Delegate: Dr. Carlo Mealli

1. Introduction

The International Union of Crystallography spreads the principles of crystallography in the field of molecular sciences and materials. Furthermore, it promotes international cooperation between researchers of different scientific backgrounds, with the common interest of establishing the three-dimensional distribution of atoms in the matter. By defining the important correlations between structure and properties, Crystallography has become an indispensable tool for all the research activities, having acquired a deep multi-disciplinary character. In about a century, amazing results have been achieved for the progress of human knowledge thanks to the knowledge of most of the matter around us. In particular, the excellence of the crystallographic approach is confirmed by the many Nobel prizes awarded to crystallographers. In the most recent decades, many functionalities of the large molecules of life have been understood thanks to their structural determination (*e.g.*, ribosomes). This has had a high impact on the health, since it is possible to fix some arisen defects in these molecule by using for instance ad hoc drugs and maintaining their vital functions.

It is important to remember that in the approximately seven decades of IUCr life, Italy has always played a proactive role. For example, it provided a president (Prof. Mario Nardelli), as well as two presidents of the associated Europeaan Crystallographic Association (ECA), such as Carmelo Giacovazzo and Alessia Bacchi. Many Italians have offered their competent contribution to the progress of IUCr and ECA. Two of the IUCr three-year congresses (with up to 3000 participants) have been organized in Italy (Rome 1961 and Florence 2005), while also two European meetings (ECM) have been assigned to Italy (Turin 1985 and the 2021 in Padua). For these and many other reasons, the Italian crystallography continues to be a cornerstone of IUCr. From the instrumentation point of view, Italian workers are well equipped, despite the country's undeniable economic difficulties. Among other things, cutting-edge equipment has recently been acquired for the Cryocrystallography in Milan (Univ.) and in Naples (IGB-CNR).

For all the mentioned reasons, the CNR representative at the IUCr (Dr. Carlo Mealli, outgoing due to age limits) leaves a solid situation of Italian crystallography. As evidence of this, we can recall the great vitality of the Italian Association of Crystallography (AIC), having Prof. G. Diego Gatta (Univ. Milano) as President. The AIC is very active at all national and international levels with congresses, schools, workshops and more.

The undersigned seizes the occasion of this last report to thank the CNR for providing a long lasting possibility of acting as the liaison with one of the most powerful world scientific Unions such as the IUCr. He also wishes his successor, Dr. Michele Saviano, a most fruitful work in the years to come.

2. Main activities carried on by (Union name) during 2018 relevant for Italy and for CNR

Over 2018, the most important event for the Italian crystallographic community was the 21rst Conference of the European Union of Crystallography, in Oviedo (Spain, 23-28 August), in which several Italian crystallographers served as chairs of micro-symposia or as speakers. In addition, the Italian community has been very active organizing congresses, schools and workshops. Among those: 1) The joint conference of the Italian Crystallographic Association and the Italian Society of Synchrotron Light, in Rome (25-28 June); 2) The AIC School in Bari (29 August – 2 September), with a relevant number of European and extra-European participants (from Albania, Algeria, Croazia, Egitto, Germania, India, Irlanda, Italia, Malesia, Marocco, Norvegia, Polonia, Romania, Russia, e Tunisia); 3) The Workshop AIC-GIDRM "CHANCES: Crystallography and NMR in Complementary Structural Investigations", in Florence (4 September). Additional activities, organised by AIC members and aimed to promote the diffusion of the crystallographic sciences, have been supported by AIC; a full list is available at: www.cristallografia.org.

It is worth remembering that the General Assembly of the Union of the XXIV IUCr congress of Hyderabad (India, 2017) proceeded to renew its governing bodies such as the Executive Committee (EC) and the members

of the 20 scientific commissions (publishing and non-publishing). As many as 20 Italians were nominated including two chairs, seven full members and thirteen consultants. Importantly, in 2018, the Italian researcher, Dr. Angela Altomare (CNR, Bari), has become co-editor of one of the fundamental newspapers of crystallography, such as Acta Crystallographica (A).

The financial situation of the Union, which had been in slight deficit in previous years, improved in 2018 thanks also to new initiatives such as the launch of IUCr Data, *i.e.* a new format for Acta E.

The IUCr Executive Committee implemented a resolution of the 2017 General Assembly, namely that of striking a prize for a distinguished young crystallographer. It was suggested that the Prize had the designation of the two Braggs, father and son. Now the texture of the reward has been established, one of the rules been that no more of ten years must have passed from the obtainment of the PhD.

The new president IUCr, Sven Lidin (Sweden), has developed in particular a new policy, appointing Andrew Allan, as the new Editor in Chief.

3. Activities carried on by (Italian Delegate name) within the Union during 2018 and impact on the Italian scientific community

It is worth emphasizing that since 2011 Italy no longer has its own representative in the IUCr's Executive Committee, so much effort has been devoted to identify the internationally renowned Italian crystallographer to be presented as a candidate for the next IUCr Congress in Paris 2020. Additionally, since also the 20 IUCr commissions must undergo some renovation, similar discussions have been held within the CNR Commission for the relations with the IUCr about the expertise of various candidates in the different areas. All the Italian proposals must be submitted during 2019, *i.e.* only short after the date of presentation of the present report.

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

The IUCr with more than 20,000 members is one of the largest scientific unions in the world and is still growing even for the accession of several new nations after the International Year of Crystallography (IYCr2014), the latest members being Albania, Kosovo, Tunisia, Singapore and Bangladesh. Other nations could be accepted in 2020 such as for instance Columbia and Thailand.

As already mentioned, the IUCr mission is the international dissemination of its basic culture and the international cooperation. Hence, it is essential that Italy continues to be part of such a vast scientific community. The cost incurred by the CNR for membership (approx. 6000 euros per year) appears to be sustainable in light of the great benefits for both from our national crystallographic community but also that of many neighboring scientific sectors, which make abundant use of the crystallographic techniques and their applications.

From the point of view of economic return, it should also be emphasized that almost all the events for crystallography organized in Italy receive some economical support from the Union, often with an advantage with respect to the paid association fees.

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

Through the activity of the Italian representative and of the CNR-IUCr Commission, as well as of the IUCr outreach officer (the Italian Michele Zema of the University of Pavia), the programs and the IUCr activity are monitored in details. In particular, the 20 Italian scholars, who are part of the 20 scientific committees of the Union receive first-hand information on the up to date research in each different sector. These persons have therefore the opportunity of reporting these pieces of information thus stimulating frontier initiatives also in our laboratories. From this point of view, the Italian Association of Crystallography (AIC) promotes in its congresses and schools the meeting between the aforementioned Italian IUCr commissioners and the world of researchers, especially the young.

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

There are numerous Italian researchers with important roles in the world of crystallography. In the ECM congress of Oviedo, Prof. Alessia Bacchi (University of Parma) ended her mandate as ECA President, remaining however in the Executive Committee as Past President. Michele Zema (University of Pavia), after various positions held in the IUCr itself, has now the fundamental role of "Outreach Officer" of the IUCr. Andrea Zappettini (CNR-IMEM of Parma) is an ex-officio member of the Executive Committee of the International Union of Crystal Growth, in which Roberto Fornari (Univ Parma) is Past President. Furthermore, Matteo Leoni (Univ Trento) is chair of the Board of Directors of the International Center for Diffraction Data

(ICDD). As mentioned, there are 20 Italian members of the IUCr commissions, with two of them being chairpersons.

7. If Union with CNR Commission, short summary about the 2017 CNR Commission activities

The CNR can count on the advices of the "Commission for the Participation of the CNR in the IUCr". With the end of 2018 the previous commission, of which the undersigned was a member, lapsed and a new one was installed, whose members nominated CNR are: Roberta Oberti (confirmed president), Michele Saviano (confirmed secretary), Gilberto Artioli, Federico Boscherini, Andrea Ienco, Andrea Ilari, Giuseppe Zanotti, Andrea Zappettini, Michele Zema and G. Diego Gatta, as the AIC President in charge. During 2018, the old commission held several teleconferences for the planning of the various activities of crystallographic interest and to prepare some remark for the new commission on some still pending matters, such as the potential appointments of Italians for the IUCr Commissions and the new EC, which will be submitted to the AG of Paris 2020, but which will have to be presented to IUCr in 2019.

Interactions with Chester's IUCr staff were also frequent, also because the outreach office Michele Zema is always available with new pieces of information and useful links.

8. Conclusions

The IUCr continues to be a vital international body for almost all scientific disciplines, in many cases playing a leading role for the international community. Its mission and aims are well illustrated on the website <code>www.iucr.org</code>. In Italy, most crystallographers are well connected not only to the IUCr's activities but also to those of the European associate ECA (<code>www.ecanews.org</code>), besides the very active national partner AIC (<code>www.crystallography.org</code>). Hence, there are many reasons why I wish recommending to the CNR not only to support the complex network of international contacts already in place, but also to better favor the most active researchers of the Italian crystallography in their efforts gaining international weigh, especially through the channels of the IUCr.

Faithfully,

Place and date:

Carlo Heall.

Sesto Fiorentino June 10th 2019