International Union of Crystallografy (IUCr)

Report on the 2017 activities

Edited by the Italian Representative at the IUCr, Dr. *Carlo Mealli* (past Research Director and Associated Researcher of CNR-ICCOM)

1. Introduction

From 1946, the IUCr has been carrying out intense and fruitful activities for the diffusion of crystallography and the promotion of international cooperation. The character is highly multidisciplinary, especially for the developments emerging from the relationships between structure and properties in many sectors of the sciences. A final example is the integration of the crystallographic approach with electron microscopy, which has led to the awarding of the 2017 Nobel Prize in Chemistry (Dubochet, Frank and Henderson) for high definition structures in the bio-molecular field. Incidentally, Italy already has a cryo-crystallography laboratory at the University of Milan, and one will soon open at the CNR_IGB in Naples. Moreover, Italian contributions to crystallography have always been significant with many scholars involved in international collaborations and the outreach activities of IUCr.

2. Significant activities for Italy and for the CNR carried out in 2017 by the Union

The major event of 2017 has been the XXIV IUCr Congress with annexed General Assembly (AG), which was held in Hyderabad, India, from August 21st to 27th. Italy has been involved in the organizational process, having three members of the International Program Committee (IPC) (G. Artioli, A. Zappettini and P. Macchi) and a member of the Local Organizing Committee (M. Zema, also as an observer of the IPC). Unfortunately, the undersigned representative, after several consecutive presences to this type of events (including the XX Congress, which he organized and chaired in 2005 in Florence), could not be present for family reasons. Also for this reason, on the proposal of the CNR-IUCr Commission, the CNR appointed the official delegation formed by the following members: Giuseppe Zanotti of the University of Padua (Head of Delegation), Federico Boscherini of the University of Bologna and Andrea Zappettini of IMEM-CNR (Parma), all members of the CNR-IUCr Commission.

3. Activities carried out as a representative in 2017 within the IUCr with repercussions on the national scientific community

The undersigned think it is useful to summarize the salient points from the report on the XXIV congress IUCr and AG, already presented to the CNR by the aforementioned official delegation in India. In fact, the congress is the most significant moment of the three-year period 2015-2017, hence it is important to disseminate its salient points to our entire national scientific community. The scientific quality has been high, as suggested for instance by the conference of Tom Blundell of the University of Cambridge, who was granted the maximum IUCr Ewald prize, as a renowned protein crystallographer and former student of Dorothu Hodgkin (Nobel laureate in 1964). Also several Italian contributions have been of primary importance. One of the most esteemed crystallographers grown in Italy, namely Giacomo Chiari (now in Los Angeles) held one of the only three plenary lectures. Four other Italians presented keynotes: Dario Braga (Bologna), Matteo Leoni (Trento), Giuseppe Resnati (Milan) and Massimo Nespolo (now in Nancy). Furthermore, the following researchers have been selected to organize and chair several microsymposites: Alessia Bacchi, Paolo Falcaro, Pierangelo Metrangolo, Mauro Gemmi, Giuliana

Aquilanti, Nicola Casati, Isabella Pignatelli, Francesco Mezzadri, Roberto Mosca, Annalisa Guerri, Michele Zema. It should also be said that the total number of presences in Hyderabad was lower than usual (1700 people with 500 Indians, against an average of about 2500 participants and 3000 in Florence-2005). Evidently the travel costs have limited the turnout, including from Italy given the only 30 participants. Despite this, Italy is one of the top 10 nations in the world in this sector. Turning to the GA, four new nations have joined the Union: Albania and Kosovo, Tunisia, Singapore and Bangladesh. In particular, the entry of Albania has been strongly supported by Italy, in particular thanks to the work of the CNR researcher Dritan Siligi (IC of Bari) with Albanian origin but active member of the Italian Association of Crystallography (AIC) since many years. Among other news in the IUCr administration, a major role continues to be played by Michele Zema (Pavia), who is a member of the CNR-IUCr Commission. For the IUCr, he managed the International Year of Crystallography (IYCr2014) and later became Outreach Officer for the diffusion of crystallography, position in which he has been reconfirmed for three more years. The creation of the new prize for young crystallographers, entitled to the two Braggs, father and son, has been proposed and discussed. The activities of the twenty IUCr commissions (publishing and non-publishing) has been analyzed in details by the GA. The commissions include several Italian researchers, including two coordinators (A. Zappettini for "Crystal growth" and G. Artoli for "Crystallography in art and cultural heritage"). Two new Italian members have been coopted into IUCr Commissions, namely B. Vallone (Biological Macromolecules) and A. Guerri (Crystallographic teaching). Next, the GA moved to the votes. First, there was a balloting between San Diego and Melbourne for the seat of the XXVI IUCr Congress in 2023, after the one in Prague 2020. Melbourne was nominated by a qualified majority. Then, there were the polls for the new Executive Committee (EC). Six candidates concurred for president (incidentally, Italy had supported the candidacy of John Helliwell, given his prestigious curriculum and excellent scientific nature). Sven Lidin (Sweden) was elected, while Hanna Dabkowska (Canada) was chosen as vice presidency and Luc van Meervelt (Belgium) as treasurer. The new EC will consist of Jennifer Martin, Graciela Diaz de Delgado and Masaki Takata, Marvin L. Hackert (Past President), Wulf Depmeier, Santiago Garcia-Granda and Radomír Kuzel. The undersigned believes that all the previous information will be particularly useful to have in order to plan the entry of an Italian representative into the future Executive Committe, since no member of ours has been coopted since 2011 (see point 4).

4. Evaluation of participation in the Union in relation to the benefits and costs of membership

The IUCr with more than 20000 members is one of the largest scientific unions in the world and is still growing for the access of several new nations after IYCr2014. The Union abounds of scientific personalities in many different sectors of the frontier research, as evidenced by the numerous Nobel laureates coming from Crystallography. Given that the IUCr mission is the dissemination of the discipline and the international cooperation, it is essential that Italy remains in the world elite, a role taken for many decades. The yearly membership to IUCr costs about 6000 euros to CNR, a sum apparently sustainable in light of the benefits for the Italian crystallography are widely exploited.

5. Evaluations on Italian participation with proposals to improve interest and involvement

Through the work of the Italian representative and the CNR-IUCr Commission, as well as the Union's Outreach Officer (M. Zema), Italy closely monitors the IUCr programs and activities within the international scientific community. As mentioned, there are many Italians who work in the 20 scientific

commissions IUCr also with the possibility of addressing the main scientific aspects. While Italy still has the presidency of the European association ECA with Alessia Bacchi (Parma), after the exit of Davide Viterbo in 2011, no other Italian has been coopted in the IUCr's EC. It is therefore important to present an adequate candidacy for the polls at the next GA in Prague - 2020. For this, some scientific personalities have to be monitored, while suitable alliances with other nations shall be pursued. The "Commission for the Participation of the CNR at the IUCr" shall work to this target and consult with the world of Italian crystallographers. It will be also important to be proactively present at the next two European congresses (ECM31, Oviedo 2018 and ECM32, Vienna 2019). For this, the CNR support will be fundamental, hence it is suggested that small official delegations are nominated and financially supported.

6. Italian experts with apical roles appointed within the organization or in commissions and related programs (of which we are aware)

Several names of Italian researchers with important roles in the world of crystallography have already appeared in this report. Prominanet names are those of Alessia Bacchi, the ECA president in charge, and Michele Zema, the powerful IUCr outreach officer. To be added, are the names of Andrea Zappettini (CNR-IMEM), ex officio member of the Executive Committee of the International Union of Crystal Growth, of which Roberto Fornari (Parma) is the Past President. Furthermore, Matteo Leoni (Trento) is Chair of the Board of Directors of the International Center for Diffraction Data (ICDD). Then, the role of the 15 Italian members in the IUCR commissions is also of primary importance for outlining for outlining the avant-garde themes of the crystallographic research, as well as for the selection of speakers in international congresses.

7. Brief summary of the 2017 activities of the CNR Commission

The CNR can count on the advices of the "Commission for the Participation of the CNR at the IUCr", active since the end of 2015 and formed by Gilberto Artioli, Federico Boscherini, Andrea Ilari, Carlo Mealli. Roberta Oberti, Michele Saviano, Giuseppe Zanotti, Andrea Zappettini and Michele Zema, with Oberti and Saviano being president and secretary, respectively. During 2017, various telematic meetings were aimed at preparing for the XXIV IUCr Congress and GA of Hyderabad, including the identification of the official CNR delegation and other requests for the congress organizing committee. As already mentioned, the commission has been active in proposing the best applications both to the IUCr governing bodies and the commissions. Interactions with Chester's IUCr staff were also frequent.

Conclusions

As a representative of the CNR at IUCr, I confirm that the Union is increasingly a vital international scientific body with a leading role for the international community. Its purposes are well illustrated on the <u>www.iucr.org</u> website. In Italy, most of the crystallographers are well connected not only to the activities of the IUCr but also of its European emanation, namely the European Crystallography Association, ECA (<u>www.ecanews.org</u>), and the Italian one, AIC (<u>www.cristallografia.org</u>). There are therefore multiple reasons for recommending to the CNR, not only the continuation of favoring the complex network of the ongoing international contacts, but also the support to the most active Italian researchers, who increase the weight of our community at the scientific Union.

Dr Carlo Mealli Carlo Heall,' Sesto Fiorentino, April 3rd 2018