

## **GIG<sub>3</sub> – Education in Crystallography**

**Reported Period: 2017-2018**

**Report Date: 29 July 2018**

**Reported by: Annalisa Guerri, Chiara Massera and Marijana Đaković**

---

### **1. Introduction.** (50 words max.)

In the last year GIG<sub>3</sub> has continued its activities in support of the educational events (ECS<sub>5</sub>) of the Association, and has provided letters of endorsements for other events (see point 10 for details). Moreover, GIG<sub>3</sub> started to work with other SIGs/GIGs for the next ECM in Vienna.

### **2. GIG web site:**

Under construction at <http://www.gig3eca.unipr.it>.

### **3. Number of ECA individual members registered with the SIG according to (<http://ecanews.org/mwp/groups/gig-03-education-in-crystallography//>)**

GIG<sub>3</sub> Education in Crystallography, 30 members

### **4. Existence of a SIG mailing list: Yes**

**Address of the mailing list:** [gig3eca@unipr.it](mailto:gig3eca@unipr.it)

**Number of members in the SIG mailing list:** 30

### **5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate).**

30

### **6. List of MS organized by the SIG at the last ECM**

One MS on "Education in Crystallography" and two MSs jointly organized, one with GIG<sub>1</sub> on "How to take your next steps in Crystallography" and one with SIG<sub>9</sub> on "Training computational method developers".

Other than the MSs, GIG<sub>3</sub> organized a special exhibition with posters from European countries highlighting the local/national teaching activities which have been carried out in the different countries. The exhibition will last for the whole period of the ECM conference.

### **7. Prizes sponsored/coordinated**

None

### **8. Past Activities other than Microsymposia at ECM**

Interaction with the Local Organizing Committee of the ECS<sub>5</sub> from South Africa, for the organization of the school

The bid for the next European School (ECS<sub>6</sub>) in 2020 will be presented to this ECM. The Hungarian colleagues contacted GIG<sub>3</sub> to have information and suggestions on how to proceed in the organization and the timeline of events needed for it.

### **9. Future/Programmed Activities**

GIG<sub>3</sub> will liaise with other Crystallography Associations and IUCr Commissions regarding their initiatives. For instance, some joint IUCr/ECA teaching pamphlets could be produced, and a newsletter could be published within the web site of the Group.

GIG<sub>3</sub> is already involved in the organization of the next ECM<sub>32</sub> in Vienna, with a representative (Annalisa Guerri) in the Programme Committee. It has been proposed to have two joint MSs, one with GIG<sub>2</sub> (Senior Crystallographers) and another one with SIG<sub>9</sub> (Crystallographic Computing) on integrative methods to characterize the structure of a compound.

**10. Other matters.** (50 words max.)

GIG<sub>3</sub> supported The Pan African Conference on Crystallography (PCCr<sub>2</sub>) which will be held in Accra, Ghana, from 28<sup>th</sup> January to 2<sup>nd</sup> February 2019, the International School on Advanced Porous Materials, Como (Italy) in June 2019, the To.Sca.Lake 3.0 International Workshop, Como (Italy), in May 2019 and the ISBC 2019 (International School on Biological Crystallization) which will be held in Granada from 26<sup>th</sup> to 31<sup>st</sup> May 2019.

**11. Brief annual activity report** (100 words max.)

A dedicated web site for GIG<sub>3</sub> is under construction, which aims at collecting and highlighting national and international events on education, as well as links to educational websites, papers and books.

GIG<sub>3</sub> was involved in the organization of the fifth European school in South Africa. Moreover, support from the GIG<sub>3</sub> have been sought by the organizers of different educational activities which will take place in Europe and in extra-European countries.

The involvement of GIG<sub>3</sub> in the ECM<sub>31</sub> resulted in three different microsymbiosia (see point 6) and an event linking all the European countries, i.e. "Education in crystallography, issued to students from first grade to university". The event has a form of a poster exhibition and will comprise at least 8 contributions.

**12. List SIG officers, name and e-mail, and specify their main function in the SIG:**

**Chair:** Annalisa Guerri ([annalisa.guerri@unifi.it](mailto:annalisa.guerri@unifi.it))

**Vice-Chair:** Chiara Massera

([chiara.massera@unipr.it](mailto:chiara.massera@unipr.it))

**Secretary:** Marijana Đaković

([mdjakovic@chem.pmf.hr](mailto:mdjakovic@chem.pmf.hr))

**Webmaster:** Fermin Otálora ([fermin@lec.csic.es](mailto:fermin@lec.csic.es))

**Board members**

Catharine Esterhuysen

([ce@sun.ac.za](mailto:ce@sun.ac.za))

Fernando J. Lahoz

([lahoz@unizar.es](mailto:lahoz@unizar.es))

John Helliwell ([john.helliwell@manchester.ac.uk](mailto:john.helliwell@manchester.ac.uk))

Fermin Otálora Muñoz

([fermin@lec.csic.es](mailto:fermin@lec.csic.es))

**Supplementary Materials**

Report on ECS<sub>5</sub>

## Report on the 5th ECS – Stellenbosch, South Africa, 8-14 July 2018

The fifth European Crystallographic School (ECS5) was held under the auspices of the European Crystallography Association (ECA), the International Union of Crystallography (IUCr) and the South African Crystallographic Society (SACrS) in Stellenbosch, 8-14 July 2018. The school was attended by 86 participants, including 21 lecturers and tutors, from thirteen different countries, primarily from Africa. The first part of the school, from 8 July to 10 July, constituted an introduction to the fundamentals of crystallography, including symmetry, space groups, diffraction physics, crystallisation and the theory behind data collection, structure solution and refinement. From 11 – 13 July the participants divided into two groups, one focusing on materials science, and the other on structural biology.

The structural biology session included a visit to the University of Cape Town on 12 July for a demonstration of the instrumentation housed in the Structural Biology group, as well as hands-on sessions on crystallisation and structure solution and refinement. The materials science grouping also focused on hands-on sessions on the Cambridge Structural Database, structure solution and refinement, powder diffraction (including Rietveld refinement) and solution of twinned and disordered structures. There was also a demonstration of the Stellenbosch University diffraction equipment. On the final day of the school the two groups joined up again for a description of how to report crystallographic data, neutron diffraction, and an overview of what crystals can be used for, followed by a final closing.

The daily programme consisted of four 1.5 hour lectures per day, separated by tea breaks and lunch, with a final discussion session at the end of the day, where students were divided into groups according to interest group and level of experience and were able to discuss the issues and questions that they had had during the day with an experienced mentor. At the end of these sessions the mentors met and discussed the questions that had arisen to determine what points required the most clarification, and feedback on these was then given at the beginning of the next day.

The social aspects of the event were also not neglected: on the opening evening of the school there was a well-attended mixer to give students the opportunity to meet each other, and the tutors and lecturers. On Wednesday afternoon there was an excursion to the wine estates Zorgvliet for wine tasting or Tokara for olive oil tasting and Spice Route, where the participants had a choice of wine, beer, gin, chocolate and charcuterie tastings. This was followed by dinner at the pizza restaurant on Spice Route wine estate. The farewell function on 13 July was a 'spitbraai' – lamb roasted on a spit – accompanied by a variety of the local wines, for which the region is world famous. These social events gave the students the opportunity to network with their peers and the lecturers and tutors involved in the school in an informal setting.

The ECS5 was funded by a number of organisations, to whom we would like to express our gratitude: the ECA for student support, the IUCr for student support and travel costs for two of our international lecturers, the Italian Crystallographic Association, the Cambridge Crystallographic Data Centre and the South African Chemical Institute for student support, Mitegen for bags (including two of their mounts), Bruker for pens and books, USB sticks, the travel costs of Tobias Stürzer and general funding, Malvern Panalytical for books on powder diffraction and general funding, Crystal Growth and Design and Wirsam Scientific for general funding, SASOL for student support and the Royal Society of Chemistry (Dalton Division) for accommodation for Andrew Bond and Ilia Guzei and printing costs. CrystEngComm donated prizes for students, and offered one-year subscriptions to all ECS5 participants who did not have access to their journal.

This funding definitely contributed to the success of the school: the feedback from the participants (both students and lecturers) has been overwhelmingly positive, with more than 80% of the students describing the school as good or excellent, and as useful for their research. The individual comments were in general also very positive, with the greatest complaint being that the lunches were too small. The lecturers and tutors involved in the school also enjoyed the experience, and remarked on the dedicated and positive attitudes of the students. Both lecturers and students had good advice for future schools, which will be passed onto the organisers of the next ECS.