

GIG-2 Senior Crystallographers

Reported Period: 2021-2022

Report Date: 6 August 2022

Reported by: Bill Clegg

1. Introduction

During the period since ECM32 in Vienna GIG-2 has been largely dormant because of Covid-19 and the vulnerability of people of this age bracket, with no ECM until ECM33 forthcoming in Versailles.

2. GIG web site:

<https://ecanews.org/groups/gig-02/> (This has not been updated for some time)

3. Number of ECA individual members registered with the GIG-2 according to

(<http://www.xray.cz/eca/im-payment.htm>)

Attempts to obtain this information from the ECA website continue to produce error messages.

4. Existence of a GIG-2 mailing list: YES

Address of mailing list: Maintained by the interim secretary, Prof. Helen Stoeckli-Evans

Number of members in the GIG-2 mailing list: ca. 85–90

The GIG-2 usually maintains communication with its members by irregular updates *via* e-mail and on its website. An e-mail update was circulated in August 2021.

5: Approximate numbers of researchers involved in the GIG-2 (please indicate the basis for the estimate)

About 80% of our members, many of whom are professionally retired, continue to be deeply involved in research and teaching, as it emerges from their recent publications and personal websites. Because of the unusual current circumstances, no update to this information from 2020 has been attempted.

6. List of MS organized by GIG-2 at the last ECM (ECM32_Vienna)

Microsymposium (jointly with GIG-3 Education) entitled: "Teaching new dogs old tricks". This attracted an audience too large for the allocated lecture room and many had to be turned away. Some of the contributions to this session have subsequently been converted to manuscript form and published in *Acta Crystallographica Section E*.

7. Prizes sponsored/coordinated.

None at present.

8. Past activities other than Microsymposia at ECM

None this year.

9. Future/Programmed Activities

ECM33: Versailles, France, 2022

Several Microsymposia have been proposed, some by GIG-2 alone, others jointly with GIG-1 and/or GIG-3. The proposals are as follows, in order of preference, and include suggestions for keynote/plenary lectures also.

1. Teaching new dogs old tricks. This was a very popular and successful MS in ECM32 so we should have another with either the same title or a different one conveying the same impression. The exact topics will, of course, not be the same but the principle will still be for experienced crystallographers to impart some of their accumulated knowledge and expertise to younger colleagues. We believe this proposal is strongly supported by GIG-1 and GIG-2.

2. Opening the black box (or So how does that work?), giving insights into how some popular programs, routines and methods work, e.g. how unit cells are automatically determined on a diffractometer, space group determination, modern structure solution techniques such as charge flipping and SHELXT, some structure refinement tricks.
 3. A session looking at past and present French contributions to crystallography (as the meeting is in France); this would probably be entirely a GIG-2 enterprise, while other proposals here will probably be supported by other GIG/SIGs.
 4. A MS on aspects of reliability in crystallography, perhaps including a basic statistics tutorial and something on validation, publication, and effective database use.
 5. What should undergraduate students learn about crystallography? This could have contributions regarding particular main subjects (physics, chemistry, biology,...). I believe a number of GIG-3 members have suggested the topic "Teaching crystallography to non-crystallographers", which amounts to much the same thing.
 6. A teaching MS on understanding and using information in Volume A of International Tables; we had a session like this specifically for young crystallographers at a BCA annual meeting a few years ago and it was very well received and appreciated.
 7. A session on the public understanding of crystallography.
- We propose that at least one plenary and/or keynote lecture should be specifically educational rather than presenting personal research. Some of the MS topics proposed above would be suitable subjects to be tackled by an experienced and eminent crystallographer.
- Another plenary or keynote lecture could be an autobiographical account by a senior crystallographer and would bring in some historical aspects of the development and activities of ECA. Perhaps one of the previous ECA Presidents as speaker?

10. Other Matters

None at present. GIG-2 will resume activities at ECM33.

11. Brief annual activity report

Until March 2020, and particularly at ECM32 in Vienna, GIG-SC continued to promote the interests of the members of the group. Greater collaboration and interaction has been sought with GIG-1 and GIG-2, particularly in joint proposals for ECM Microsymposia and exploring the possibility of other common interests. This has been successful in respect of ECM33 Microsymposia, and a joint meeting of GIG-1 and GIG-2 during ECM33 is proposed (the two GIG meetings are scheduled simultaneously so that the groups can come together at the end of their individual discussions).

GIG-2 has been involved, together with GIG-1 and GIG-3, in the planning of the following MS at ECM33:

MS45: What is inside the black box?

MS46: Reproducibility in crystallography

MS47: New horizons in teaching crystallography in the 21st century

MS48: What should undergraduate students learn about crystallography?

Together with the ECA 25th and ECM 50th anniversaries celebration before the conference dinner.

12. GIG officers, name and e-mail, and specify their main function in the GIG.

Committee

Chair:	Bill Clegg	bill.clegg@ncl.ac.uk
Co-Chair:	Vacant, to be appointed	
Secretary:	Helen Stoeckli-Evans	helen.stoeckli-evans@unine.ch

Webmaster: Helen Stoeckli-Evans helen.stoeckli-evans@unine.ch

Officers:

George Ferguson gf3@st-andrews.ac.uk

Ton Spek a.l.spek@uu.nl

Enrique Gutierrez Puebla egutierrez@icmm.csic.es

It was intended to find new Co-Chair, Secretary and Webmaster during the 2020 IUCr Congress in Prague, but this had to be postponed and will take place at ECM33. Bill Clegg is willing to continue as Chair of GIG-2.