GIG-2 Senior Crystallographers Reported Period: 2019-2020 Report Date: 1 February 2021

Reported by: Bill Clegg

1. Introduction

GIG-2 jointly organized a Microsymposium with GIG-3 at ECM32 in Vienna. This was a great success, with an over-capacity audience. During the period since March 2020 GIG-2 has been dormant because of Covid-19 and the vulnerability of people of this age bracket.

2. GIG web site:

https://ecanews.org/groups/gig-02/

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 produced 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.* 88

The GIG-2 usually maintains communication with its members by irregular updates *via* e-mail and on its website, but there has been nothing to report during the last year.

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 last year 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, 2021 (?)

Several Microsymposia have been proposed, some by GIG-2 alone, others jointly with GIG-1 and/or GIG-3. Decisions on the programme have not yet been made. 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 when Covid restrictions allow greater freedom.

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.

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 as soon as possible at the next available meeting (Congress or ECM).