European Crystallographic Association Reports of the Executive Committee & Reports of the Special/General Interest Groups September 2011 - June 2012

Report of SIG 9

SIG No:

Reported Period: 2011-2012

Report Date: 18/05/2012 Reported by: Harry Powell

1. Introduction. (50 words max.)

Finally we have a website - very basic at the moment, but can now be populated with news etc. A Deputy Chairman has been appointed, and two people have agreed to serve on the Committee. Following my retirement as Chairman of IUCr CompComm, I have been able to devote more time to SIG9. We should start a search for a logo.

2. SIG web site:

SIG 9 url: http://sig9.ecanews.org/

3. Number of ECA individual members registered with the SIG according to

(http://www.xray.cz/eca/im-paymenthtm)

SIG 9 ecacomsig number

4. Existence of a SIG mailing list O Yes / O No

No (an informal list is kept by

92

HRP; a list is held on IUCr web server but does not seem to elicit any replies)

Address of the mailing list:

Number of members in the SIG mailing list:

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate) ~200 based on the mailing list and knowledge that most researchers in this field are not on the list.

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

MS44 Software development, automation and validation at ECM26. 8 MS at IUCrXXII in Madrid co-organised with IUCr CompComm. Computing School held before IUCrXXII in Oviedo, Spain organised by SIG9 members in role as CompComm members, attended by ~55 people.

7. Prizes sponsored/coordinated

None at present. A competition will be held for one free registration to ECM28 (open to young members, with some further restrictions, e.g. resident in an economically disadvantaged country).

8. Past Activities other than Microsymposia at ECM

none this year

European Crystallographic Association Reports of the Executive Committee & Reports of the Special/General Interest Groups September 2011 - June 2012

Report of SIG 9 (cont.)

For Each Activity

Title:

Number of Participants:

Level of involvement of SIG in the activity:

O ECA Individual Members registered with the SIG involved in the organizing committee

O ECA Individual Members registered with the SIG involved as lecturers

O endorsed (SIG logo on the web page/leaflets)

Sponsored by ECA?

OYes/ O No

Other Sponsors/Organizers:

Short Description: (50 words max.)

9. Future/Programmed Activities.

For Each Activity

Title: Software Fayre at ECM27

Number of Participants: 15 - 20 in each of 6 sessions

Level of involvement of SIG in the activity:

O ECA Individual members registered with the SIG involved in the organizing committee 1

O ECA Individual members registered with the SIG involved as lecturers 4 - 6

O endorsed (SIG logo on the web page/leaflets) no

Sponsored by ECA?

OYes/ O No don't know

Other Sponsors/Organizers: don't know

Short Description: (25 words max.)

Workshops based on use of ~6 different software packages.

Title: Crystallographic Computing workshop (prior to ECM28)

Number of Participants: 15 - 20

Level of involvement of SIG in the activity:

O ECA Individual members registered with the SIG involved in the organizing committee 2

O ECA Individual members registered with the SIG involved as lecturers ~5

O endorsed (SIG logo on the web page/leaflets) yes

Sponsored by ECA?

OYes/ O No Haven't applied yet

Other Sponsors/Organizers: Should be able to find 3 - 6 sponsors

Short Description: (25 words max.)

Likely to be based on the use of cctbx/smtbx and other libraries/toolboxes in developing software for crystallography.

10. Other matters. (50 words max.)

I intend to retire at ECM27, so will be looking for a successor.

Report of SIG 9 (cont.)

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

Organised 4 MS for ECM27. Martin Lutz (in his own capacity) organised a Software Fayre to be held at ECM27.

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

Chairman - Harry Powell, harry@mrc-lmb.cam.ac.uk or hrp1000@cam.ac.uk

Deputy Chairman - Martin Lutz, m.lutz@uu.nl

Committee: Laura Roces, laura.uniovi@gmail.com

Andrea Thorn, andrea.thorn@WEB.DE

Supplementary Materials.

(List of all supplementary materials, if any, related to the SIG report)

3. Addendum 1 to n (to be sent in separate files)