



SIG13

Reported Period: June 2011 – June 2012

Report Date:

Reported by: Andreas Roodt (SIG Chair)

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1. Introduction. (50 words max.)

During the last year the SIG13 committee has continued to reorganise and promote the SIG to the structural science community, participating actively in the ECM27 Bergen meeting and in the organization of the past IUCr 2011 Madrid congress. The excellent results obtained in the involvement in the organization of the past IUCr 2011 meeting has resulted in a successful workshop in which several young scientists have been involved. During the IUCr 2011 Madrid congress, after a stimulating meeting between members of the SIG13, the new SIG Officers have been elected. In continuity with the previous team, Prof. Andreas Roodt has been selected as new SIG13 Chair, while the co-chair and secretary remain the same.

SIG13 representatives have been active in the development of the programme for the Bergen meeting and have made major contributions to the setting up of 12 Microsymposia. They have selected the topics and chosen the microsymposia chairs. To cover the breadth of the subject some of the microsymposia have been organised jointly with SIG7.

2. SIG web site:

SIG13 <http://sig13.ecanews.org/>

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

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

SIG13 Molecular Structure and Chemical Properties 145

4. Existence of a SIG mailing list Yes / No

Address of the mailing list: <http://www.facebook.com/pages/ECA-SIG13/137466489407#!>

Number of members in the SIG mailing list : 20

The ECA-SIG13 facebook home page has enabled the promotion and advertisement of all events related to our activities.

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate) 110 from ECA registration but additional contacts through French, British, Italian and Spanish Crystallographic Associations.

6. List of MS organized by the SIG (also in collaboration with other SIGs) at the ECM27 in Bergen.

Intermolecular interactions at ambient and extreme conditions (MS23)

Polymorphism and chirality in molecular crystals (MS24)

Porous materials for gas storage and other applications (MS26))

Molecular structures in catalysis and magnetism (MS27)



Report of SIG 13 (cont.)

Structure prediction for crystalline and amorphous molecular solids (MS40)

Dynamics in crystals: experimental techniques and software (MS41)

Big "small molecules" and small "macromolecules" – learning techniques from each other (MS42)

Hot topics and structures in molecular chemistry (MS43)

Prizes sponsored/coordinated

none

8. Past Activities other than Microsymposia at ECM

For Each Activity

Title: Workshop2 within XXII Congress IUCr2011 Madrid, 23-30 August

Number of Participants: around 50

Level of involvement of SIG in the activity:

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

2 ECA Individual Members registered with the SIG involved as lecturers

endorsed (SIG logo on the web page/leaflets)

Sponsored by ECA? Yes

Other Sponsors/Organizers: ECA/National Associations/ Usual Commercial Sponsors

Short Description: This workshop, proposed by the ECA Special Interest Group 13 (SIG13), organized in collaboration with the General Interest Group of Young Crystallographers (GIG-YC), and supported by the IUCr Commission of Structural Chemistry has encouraged exchanges of current experiences between different groups working in this area. Young researchers (under 35 years of age) explained with short talks (~ 20 min) to other participants the main objectives of the research carried out in their groups and on the specific research they are personally involved in. The main goal was to learn through these short talks the current work carried out on the binomial 'Molecular Structures/Chemical Properties' in different groups. We would like to stimulate the establishment of future collaboration, perhaps within the framework of international funding systems.

9. Future/Programmed Activities.

For Each Activity

Title: Workshop on basic crystallography

Number of Participants:

Level of involvement of SIG in the activity:

3 ECA Individual members registered with the SIG involved in the organizing committee

2 ECA Individual members registered with the SIG involved as lecturers

endorsed (SIG logo on the web page/leaflets)

Sponsored by ECA?

Yes

Other Sponsors/Organizers:

IUCr; Wits University, Johannesburg, and the Univ of the Free State, Bloemfontein, South Africa



Report of SIG 13 (cont.)

Short Description: (25 words max.)

A short workshop (8-10 Sept 2012) on introductory crystallography is planned at Wits University following INDABA7, 2-7 Sept 2012 (Skukuza, Kruger National Park, South Africa). Lecturers are prof D Levendis, Dr M Fernandez and Dr A Lemerer.

10. Other matters. (50 words max.)

SIG13 is continuing in the promotion of the structural chemistry at all levels, participating in “crystallographic schools” across the European Economic Community. Members will also participate in the Networks and Programmes set up by the European Research Council (and some of the national Research Councils) with the aim to provide a better understanding of structure/property relationships in solid state materials.

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

The SIG13 Committee has worked actively on the two main goals within its remit: (i) the promotion of “Molecular Structure and Chemical Properties” through greater publicity for the SIG, particular through its new website; (ii) the establishment of the Steering Committee, a list of reference scientists, one for each country within the European Crystallographic Community, to be responsible for the dissemination of events (reported above); (iii) by participating effectively in the planning process for the upcoming ECM and IUCr Meetings in Crystallography.

A specific target is the young scientists, with whom more interaction is planned.

The SIG Committee has met at the ECM and has corresponded regularly by e-mail, and has encouraged participation of SIG members at relevant national and international meetings. There has also been regular exchange of information between the SIG and officers of the IUCr Commission for Structural Chemistry to the benefit of both organisations.



Report of SIG 13 (cont.)

Steering Committee

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Report of SIG 13 (cont.)

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

- * *Chair:* Prof. Andreas Roodt (responsible for the general coordination of the SIG, and specially for interacting with the steering committee)
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- * *Co-chair:* Prof. Paul R. Raithby (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)
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- * *Secretary:* Prof. Alessandra Crispini (responsible for the SIG web-page and for maintaining the SIG member list)
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Supplementary Materials.

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

- Addendum 1 to n (to be sent in separate files)