

SIG13

Reported Period: September 2009 - June 2010

Report Date: 29th June 2010

Reported by: Fernando J. LAHOZ (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, and the number of registered SIG members has increased significantly from previous years. The SIG has been actively involved in the planning for the Darmstadt and the Madrid Meetings.

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 110

4. Existence of a SIG mailing list Yes

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

Number of members in the SIG mailing list : 13

We are trying to adopt an innovative way to join together the SIG13 members, that is the use of a social network such as facebook. Through the ECA-SIG13 facebook home page is possible to associate easily to this group meeting and participate into discussions and communications. Moreover, all events related to our activities are promptly published and every member can be easily informed and eventually join the event. Obviously, we need to advertise more the existence of this facility and encourage people that a judicious use of facebook could help a scientific community to share in real time informations and opinions.

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 at the last ECM

FA4 MS04 – Supramolecular Architectures: From Structure to Function

FA4 MS05 – Structure and Reactivity in Molecular crystals by Crystallographic, Spectroscopic and Computational Methods

FA4 MS06 – Structure and Reactivity in Metal Complexes

FA4 MS07 – Weak Interactions in Chemical Processes or Properties

FA4 MS08 – Metal Organic Frameworks – A Way Through Pores and Holes

FA4 MS09 – Crystallography in Pharmaceutical Sciences

FA4 MS10 – Indirect Structural Information: Use of Data Bases

In collaboration with other SIGs:

FA4 MS1 – Organic and Inorganic Modulated Crystal Structures

FA4 MS3 – Multicomponent Crystals

FA4 MS12 – The Future of Small Molecule Software

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymposia at ECM

For Each Activity

Title: *Associazione Italiana di Cristallografia, XXXVIII Congresso, Salerno September 20-23th 2009*

Number of Participants: 120

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: AIC/Oxford Diffraction/Rigaku/Bruker/Panalytical/Hamilton

Short Description: (50 words max.) This was the annual Italian Crystallographic Association Meeting, organized in eight microsymposia, two of which related to SIG13: MS1 “Weak interactions: the supramolecular chemist’s tool kit” and MS8 “ Structure/properties relationships in complex molecular systems: the multi-technique approach”. The Meeting included plenary lectures from international speakers but also lectures from students and extensive poster sessions.

Title: *4th Crystallographic School: Structural Analysis Using Single-Crystal X-ray Diffraction and Crystallography under Constrains, Pont á Mousson, 5-9 October 2009.*

Number of Participants: 70

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: Université Nancy / French National Reseach Council (CNRS)/Bruker/IUCr/ Oxford Diffraction and other local sponsors

Short Description: (50 words max.): This was a classical school addressed to the chemical community using single crystal experiments to characterize chemical and physical properties. Lectures were coming from France, UK, Spain and Holand

Title: *IUPAC Workshop on Halogen bonding, Milano May 7th, 2010*

Number of Participants: around 50

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: commercial sponsors: None

Short Description: (50 words max.): A workshop about intermolecular interactions involving halogens as electrophilic species. SIG13 has been involved both in the sponsorship of the workshop creating a special event on facebook and in the organization with members in the organizing committee.

Title: *Methods Complementary to Crystallography*

Number of Participants: 80

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: BCA & Rigaku Sponsored/Chemical Crystallography Group

Short Description: (50 words max.) The meeting consisted of a series of lectures where physical methods complementary to chemical crystallography had been used to solve structural problems. The speakers ranged from leaders in the field to research students.

Title: *Bill Clegg Symposium*

Number of Participants: 50

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: University of Newcastle/University of Newcastle

Short Description: (50 words max.) The meeting consisted of a series of lectures on aspects of structural chemistry given by colleagues and former students of Professor Clegg, outlining his contributions to chemical crystallography and the use of synchrotron radiation in structural determinations.

Title: *Workshop on Weak Interactions in Crystals, Universit of Alcalá, 23-25th June 2010.*

Number of Participants: 20

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: University of Alcalá/Spanish Crystallographic Association/La Factoria Project

Short Description: (50 words max.) The workshop was addressed to the Spanish crystallographic community to make them familiar with the recognition of weak interactions in the crystallographic studies, and to help them in the interpretation of properties from the structural parameters. The workshop was structured on three days including lectures and practical sessions.

Title: *British Crystallographic Association Spring Meeting*

Number of Participants: 276

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: BCA/Oxford Diffraction/Rigaku/Bruker

Short Description: (50 words max.) This was the annual British Crystallographic Association Meeting, about one third of which was devoted to "small molecule" crystallography, and symposia were covered by the general title "Data matters". The Meeting included plenary lectures from international speakers but also lectures from students and extensive poster sessions.

Title: *Master on Crystallography and Crystal Growth*

Number of Participants: 25

Level of involvement of SIG in the activity:

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

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: Spanish National Research Council/La Factorial Project/UIMP University

Short Description: (50 words max.) This is an international official Master run by the Spanish National Research Council and the International University Menendez-Pelayo. It is organized with

a 60 ECTS dedication with a reduced number of international students, and more than 40 lectures from all over the world. It is structured in three modules: a compulsory module with the basics of crystallography and crystal growth, a practical module of 20 ECTS to be done in different labs all along Europe and a third module of specialized courses. The SIG13 members are involved in the organization and as lectures.

9. Future/Programmed Activities.

For Each Activity

Title: *MISCA 2010, 2nd Meeting of the Italian and Spanish Crystallographic Associations, June 30th – July 3rd*

Number of Participants: around 200

Level of involvement of SIG in the activity:

- ECA Individual members registered with the SIG involved in the organizing committee
- 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: (25 words max.) SIG13 has been involved in the organization of the microsymbosia on Structural Chemistry and suggested plenary speakers. SIG13 members will be contributing to the Meeting by organising and speaking at several microsymbosia.

Title: *ECM26*

Number of Participants: over 700(?)

Level of involvement of SIG in the activity:

- ECA Individual members registered with the SIG involved in the organizing committee
- 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/Commercial Sponsors

Short Description: (25 words max.) SIG13 has been involved in the planning of the ECM26 Meeting and has obtained 13 microsymbosia and 2 plenary speakers. SIG13 members will be contributing to the Meeting by organising and speaking at several microsymbosia.

Title: *IUCr Congress Madrid (2011)*

Number of Participants: over 3000

Level of involvement of SIG in the activity:

- ECA Individual members registered with the SIG involved in the organizing committee
- 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/ECA/National Associations/Industrial Sponsors

Short Description: (25 words max.) SIG13 members have been involved in the planning of the IUCr Meeting at all levels, there being representatives on the Organising Committee and on the Programme Committee.

Title: *13th BCA/CCG Intensive Teaching School, Durham, UK (March-April 2011)*

Number of Participants:50

Level of involvement of SIG in the activity:

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

O ECA Individual members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: BCA/EPSRC/Industrial Sponsors

Short Description: (25 words max.) This is the 13th running of the world famous Intensive Crystallography School, held at Durham. SIG13 members are on the organising committee and will be contributing to the school by giving some of the lectures.

Title: ***British Crystallographic Association Spring Meeting (April, 2011)***

Number of Participants: 250-300

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

Sponsored by ECA? No

Other Sponsors/Organizers: BCA/Industrial Sponsors

Short Description: (25 words max.) This is the British Crystallographic Association Annual Meeting where, as usual, there will be a strong contribution from SIG13 members, who are on the organising committee and would will be planning and presenting some of the lectures.

10. Other matters. (50 words max.)

SIG13 will continue to promote 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) to develop structural methods and provide a better understanding of structure/property relationships in solid state materials.

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

The SIG13 Committee has concentrated on the two key areas within its remit: (i) the general promotion of “Molecular Structure and Chemical Properties” through greater publicity for the SIG, particular through its new website, the construction of which is nearing completion, and (ii) by participating effectively in the planning process for the upcoming ECM and IUCr Meetings in Crystallography.

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.

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

* *Chair:* Prof. Fernando J. Lahoz (responsible for the general coordination of the SIG, and specially for interacting with the steering committee)

E-mail: lahoz@unizar.es

Address: Instituto de Ciencia de Materiales de Aragón (ICMA)
Dpto. Química Inorgánica, Facultad de Ciencias
Universidad de Zaragoza-CSIC
50009 Zaragoza (SPAIN)
(Tel: +34 976 761147; Fax: +34 976 761187)

* *Co-chair:* Prof. Paul R. Raithby (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)

E-mail: p.r.raithby@bath.ac.uk

Address: Department of Chemistry

University of Bath
BATH BA2 7AY U.K.
(Tel: +44 (0)1225 383183 (direct line); Tel: +44 (0)1225 386444 (secretary);
Fax: +4 (0)1225 386231)

* *Secretary:* Prof. Alessandra Crispini (responsible for the SIG web-page and for maintaining the SIG member list)

E-mail: crispini@unical.it

Address: Dipartimento di Scienze Farmaceutiche
Edificio Polifunzionale
Universita della Calabria
87030 Arcavacata di Rende (CS), Italy
(Tel: +39 0984 492888 Fax: +39 0984 492067)

Supplementary Materials.

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

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