

**SIG7**

**Reported Period: 2011-2012**

**Report Date: 1 June 2012**

**Reported by: Susan Bourne(Co-chair) & Paola Gilli (Secretary)**

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**1. Introduction.** (50 words max.)

Established in 1999 as SIG #7, MIRSIG (Molecular Interaction & Recognition) covers the complete spectrum of theoretical, general and applicative fields of MIR. Activity includes organising dedicated sessions at ECMs and specialist meetings, workshops and schools. Because of its interdisciplinary nature, MIRSIG has established collaboration with SIG #1 (Macromolecular Crystallography), SIG #2 (Charge, Spin and Momentum Densities) and SIG #13 (Molecular Structure and Chemical Properties) to organise ECM microsymbosia.

**2. SIG web site:**

SIG7              NO (still)

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

SIG7   Molecular Interaction and Recognition                              approximately 100

**4. Existence of a SIG mailing list : No**

**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)**

The total number of researchers involved in the MIRSIG activities is difficult to estimate, but attendance at microsymbosia organised by SIG #7 tends to be between 70 and 200.

The number of ECA individual members registered with SIG #7 is 102, though we send announcements to a list of some 250 scientists working in the field. We will try to reduce this discrepancy in the near future by sending dedicated announcements to our members. Awaiting for more precise measurements, we would suggest an estimated number of 180-200 active members.

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

At the **ECM26** (Darmstadt, 29 August-02 September 2010) MIRSIG has promoted:

one Keynote Lecture:

- KL1. Jürg Hulliger: "Symmetry breaking in complex molecular assemblies" and eight Microsymbosia (out of which five in collaboration with other SIGs):
- FA1-MS6 - Molecular recognition (with SIG 1)  
(Chair: Gerhard Klebe - Co-chair: Gerlind Sulzenbacher)
- FA4-MS26 - Molecular interactions in crystal packing and molecular assemblies  
(Chair: Carl Henrik Görbitz - Co-chair: Kersti Hermansson)
- FA4-MS27 - Molecular interactions in nanocrystalline, disordered and amorphous compounds (Chair: Martin Schmidt - Co-chair: Hans-Beat Bürgi)
- FA4-MS28 - Applications of molecular crystals simulations  
(Chair: Graeme Day - Co-chair: Bartolomeo Civalieri)
- FA4-MS29 - Inclusion compounds and porous materials (with SIG 13)  
(Chair: Israel Goldberg - Co-chair: Catherine Esterhuysen)

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- FA4-MS30 - From hydrogen to halogen bonding: proton- against charge-transfer interactions (with SIG 13) (Chair: Kari Rissanen - Co-chair: Giuseppe Resnati)
  - FA4-MS31 - Supramolecular assemblies and crystal engineering (with SIG 13) (Chair: Jonathan W. Steed - Co-chair: Attila Benyei)
  - FA4-MS35 - Transformation in crystals: from polymorphism to solid-state reactivity (with SIG 13) (Chair: Demi Levendis - Co-chair: Teresa Calvet)
- and one practical workshop:
- FA4-MS32 - Crystallization in gels – a practical workshop (Chair: Juan Manuel García Ruiz - Co-chair: Jose Antonio Gavira)

The high number of joint microsymbiosia, which has been prompted by the ECA Council as well as by many MIRSIG members, has increased the number of scientific sessions organized by our SIG with respect to the past, and we take the occasion to thank the Chairman of ECM26, Professor Hartmut Fuess, for the space granted to MIRSIG subjects within this meeting.

Most of these joint activities are located within the Focus Area 4 (Chemical Crystallography), i.e. in collaboration with SIG 13 (Molecular Structure and Chemical Properties), though our long lasting cooperation with SIG 1 (Macromolecular Crystallography) is going on.

Because of the multidisciplinary nature of MIR studies, in the future we plan to start new collaborations (or to renew old ones) with SIGs of other Focus Areas. However, we have to remark that since collaborative activities increase the global complexity of the meeting, any improvement will be obtained at the cost of a greater effort not only in the program definition, but also in its scheduling.

As for the number of participants, we are pleased to say that, despite some overlaps in the timetable, both the plenary lecture and the microsymbiosia were attended by a wide audience, which testifies the interest of the European crystallographic community for MIR studies.

### 7. Prizes sponsored/coordinated

### 8. Past Activities other than Microsymbiosia at ECM

Although the SIG is not officially involved in the definition of the programme, many MIRSIG members were actively involved in the organization and running of the *XXII Congress and General Assembly of the IUCr* (Madrid, 22-30 August 2011). Some ten chairpersons and five keynote lecturers were included in the programme as well as a number of other MIRSIG members among the speakers.

Title: ***Categorizing Halogen Bonding and other Noncovalent Interactions Involving Halogen Atoms***

20-21 August 2011, Sigüenza (Spain)

Number of Participants: Limited to 50 by the organizers

Level of involvement of SIG in the activity:

O ECA Individual members registered with the SIG involved in the organizing committee Prof. Pierangelo Metrangolo (Chairman), Prof. Giuseppe Resnati (Chairman), Dr. Tullio Pilati, Dr. Giancarlo Terraneo

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Report of SIG 7 (cont.)

ECA Individual members registered with the SIG involved as lecturers  
Prof. Christer Aakeröy, Prof. Lee Brammer, Prof. Gautam R. Desiraju, Prof. Enrique Espinosa, Dr. Catharine Esterhuysen, Prof. Kari Rissanen, Dr. Giancarlo Terraneo  
endorsed (SIG logo on the web page/leaflets) No

Sponsored by ECA? No

Other Sponsors/Organizers: IUPAC, Politecnico di Milano

Short Description:

The objective of this workshop, organized as a satellite event to the IUCr 2011 Congress, was to gather several international leaders in the field around the task of giving a modern definition of halogen bonding that takes into account all current experimental and theoretical pieces of information on both gaseous and condensed halogen-bonded systems in chemistry and biology.

Title: ***XIII International Seminar on Inclusion Compounds (ISIC 13)***

12-16 September 2011, Mazurian Lakes region (Poland)

Number of Participants: 150-200

Level of involvement of SIG in the activity:

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

Prof. Janusz Lipkowski

ECA Individual members registered with the SIG involved as lecturers

Unknown at this stage

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

Sponsored by ECA? No

Other Sponsors/Organizers: PAN Chemistry Committee

Short Description:

The chemistry of inclusion compounds spans a wide area of MIR studies and ISIC represents an outstanding scientific event in this field. The main objective of this conference series, held every two years, is to present the frontiers of supramolecular chemistry as well as bring together young and experienced scientists from around the world to establish fruitful collaboration.

Title: ***Polish Summer School on Crystallography***

5-11 September 2011, Mazurian Lakes region (Poland)

Number of Participants: Approximately 80

Level of involvement of SIG in the activity:

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

Prof. Janusz Lipkowski

ECA Individual members registered with the SIG involved as lecturers

Unknown at this stage

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

Sponsored by ECA? No

Other Sponsors/Organizers: PAN Crystallography Committee, Polish Society of Crystallography

Short Description:

This edition of the traditional Polish Summer School of Crystallography was dedicated to "Chemical Crystallography in the 21<sup>st</sup> Century". Organized in the frame of the *IYC 2011* and *MSC-100* celebrations, will bring together lecturers and participants from abroad with the lively Polish crystallographic community.



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Report of SIG 7 (cont.)

Title: **Chemistry in the XXI Century – Supramolecular ?**

26-27 November 2011, Warsaw University, Warsaw (Poland)

Number of Participants: Approximately 150

Level of involvement of SIG in the activity:

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

Prof. Janusz Lipkowski

ECA Individual members registered with the SIG involved as lecturers

Unknown at this stage

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

Sponsored by ECA? No

Other Sponsors/Organizers: PAN Chemistry Committee, Warsaw University

Short Description:

This conference about supramolecular chemistry took place during the *MSC-100* closing ceremony at the Royal Castle in Warsaw. Honorary Chairman of the Symposium is the Nobel laureate in Chemistry 1987, Professor Jean-Marie Lehn.

Last but not least, we are pleased to say that some MIRSIG members were involved as organizers and participants in the conference entitled “*Women in Science*”, a special event organised on 25 November 2011 in the Royal Castle of Warsaw within the scope of the closing ceremonies of *MSC-100*. Honorary Chairperson of the Symposium is the Nobel laureate in Chemistry 2009, Professor Ada Yonath.

## 9. Future/Programmed Activities.

Title: **ECM27**

7-12 August 2012, Bergen (Sweden)

Organizing Committee: Karl Wilhelm Törnroos (Chair), Carl Henrik Görbitz

(Cochair)

MIRSIG is preparing a number of suggestions for microsymbiosia and plenary lectures to be held at ECM27. All MIRSIG members will be invited by e-mail to the MIRSIG Assembly (that will take place in Madrid during the IUCr 2011 Congress) to give their active contribution to the scientific programme of the next ECM.

Microsymbiosia at ECM27 sponsored or co-sponsored by SIG7:

**MS23 - Intermolecular interactions at ambient and extreme conditions**

Chair: Elena Boldyreva - Co-chair: Andrzej Katrusiak

**MS26 - Porous materials for gas storage and other applications**

Chair: Len Barbour - Co-chair: Alessia Bacchi

**MS24 - Polymorphism and chirality in molecular crystals (with SIG 13)**

Chair: Ulli Englert - Co-chair: Luigi Nassimbeni

**MS25 - Design, structure, and function of multi-component crystals (with SIG 13)**

Chair: Petra Bombicz - Co-chair: Laszlo Fabian

**MS40 - Structure prediction for crystalline and amorphous molecular solids (with GIG)**

Chair: Martin Schmidt - Co-chair: Aurora Cruz-Cabeza

Report of SIG 7 (cont.)

**MS12 - Molecular recognition** (with SIG 1)

Chair: Maria Carrondo - Co-chair: Annabelle Varrot

**MS33 - Neutrons and high-resolution X-ray diffraction for bio-crystallography** (with SIG 1 and SIG 6) Chair: John Helliwell - Co-chair: Matthew Blakeley

Title: ***CUSO Summer School 2012: "Hydrogen Bonding: From Gas-Phase Dimers to Biomolecular Systems and Crystals"***

August 2012 (2<sup>nd</sup> half; 5 days), Villars sur Ollon (Switzerland)

Number of Participants: Limited to 50 by the organizers

Level of involvement of SIG in the activity:

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

Prof. Piero Macchi

ECA Individual members registered with the SIG involved as lecturers

Prof. Elena Boldyreva, Prof. Gastone Gilli

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

Sponsored by ECA?

Possibly (application will be made)

Other Sponsors/Organizers: University of Bern, CUSO (Conférence Universitaire de Suisse Occidentale)

Short Description:

This summer school addressed to doctoral and postdoctoral students aims to cover modern aspects of hydrogen bonding, starting from H-bonding in dimers and extending to oligomers, crystalline solids, liquids, and biomolecular systems. The speakers are chosen to represent current H-bond research in the theoretical, general and applicative areas.

Title: ***Indaba 7, 2012***

August-September 2012, South Africa

Number of Participants: anticipated to be limited to 120

Level of involvement of SIG in the activity:

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

Prof. Leonard J. Barbour (Chairman), Prof. Susan Bourne, Dr. Catharine Esterhuysen

ECA Individual Members registered with the SIG involved as lecturers:

unknown at this stage

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

Sponsored by ECA? Possibly (application will be made in 2011)

Other Sponsors/Organizers: IUCr, South-African Universities and scientific organizations unknown at this stage

Short Description: (25 words max.)

The next in this successful series of meetings considering all aspects of molecular processes in the solid state, Indaba 7 is likely to move away from the Kruger Park. Venues near Cape Town are currently under consideration. An organising committee has been established and an advisory committee is being set up. Exact date, location and subject will be announced soon.

**10. Other matters.** ( 50 words max.)



## Report of SIG 7 (cont.)

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

During the period 2010-2011 SIG 7 has been actively involved in its prime purpose – to organise discussions, sessions and microsymbiosia relating to molecular interactions and recognition processes at a variety of conferences around the world and within the ECA annual meetings. The committee of officers recognises the need for a SIG 7 mailing list and website which could act as a permanent point of contact among MIRSIG members, but pressure of work has not yet allowed them the time to arrange these important tools and is presently working on the matter.

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

Elected during ECM25 (Istanbul) in August 2009. Office bearers from 2009-2012 are

Chairman: Susan Bourne (Cape Town) <susan.bourne@uct.ac.za>

Co-Chairman: Carl-Henrik Gorbitz (Oslo) <c.h.gorbitz@kjemi.uio.no>

Secretary: Paola Gilli (Ferrara) <paola.gilli@unife.it>

### **Supplementary Materials.**

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