

## **SIG 7 – MIRSIG (Molecular Interaction & Recognition)**

**Reported Period: 2012-2013**

**Report Date: August 2013**

**Reported by: Paola Gilli (Secretary)**

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### **1. Introduction.**

Established in 1999 as SIG #7, MIRSIG (Molecular Interaction & Recognition) covers the complete spectrum of theoretical, general and applicative fields of MIR. Activity includes organizing 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), SIG #13 (Molecular Structure and Chemical Properties) and GIG #1 (Young Crystallographers) to organize ECM microsymposia.

According to the ECA rules for the election of SIG officers, the Assembly of MIRSIG members, held on 7 August 2012 in Bergen during ECM27, has elected for the next three years the following MIRSIG Board:

Chairman: Carl Henrik Görbitz (University of Oslo) <c.h.gorbitz@kjemi.uio.no>  
Co-Chairman: Graeme Day (University of Southampton) <G.M.Day@soton.ac.uk>  
Secretary: Paola Gilli (University of Ferrara) <paola.gilli@unife.it>

The new Board expresses gratitude to the Past-Chairman, Professor Susan Bourne, for her brilliant and efficient coordinator activity during the years 2009-2012, and invites her to contribute to the future MIRSIG activities in quality of consultant.

### **2. SIG web site:**

SIG7 NO (in preparation)

### **3. Number of ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)**

SIG7	Molecular Interaction and Recognition	148
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### **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 ECM microsymposia organized by SIG #7 tends to be between 70 and 200.

The number of ECA individual members registered with SIG #7 is 148, though we send announcements to a list of some 250 scientists working in the field. We are working to reduce this discrepancy by sending announcements to our members and trying to increase the number of young crystallographers. Awaiting for more precise measurements, we would suggest an estimated number of about 200 active members.

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

At the **ECM27** (Bergen, 7-12 August 2012) MIRSIG has promoted:  
one Keynote Lecture:

- KL1. Paola Gilli: "Towards the unification of intermolecular forces: The hydrogen bond as a charge-transfer interaction"
- and seven Microsymposia (out of which five in collaboration with other SIGs):
- 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 1)  
(Chair: Martin Schmidt - Co-chair: Aurora Cruz-Cabeza)
  - 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)

We are glad to say that both the plenary lecture and the microsymposia were very well attended, which testifies the interest of the European crystallographic community for MIR studies. We take the occasion to thank the Chairman and Co-chairman of ECM27, Professors Karl Wilhelm Törnroos and Carl Henrik Gorbitz, for the space granted to MIRSIG subjects, as well as the Chairpersons and all the members of GIG #1, SIG #1 and SIG #13 that have contributed to the organization of the joint microsymposia.

## 7. Prizes sponsored/coordinated

## 8. Past Activities other than Microsymposia at ECM

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

20-24 August 2012, 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? No

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: "Insights from Structure"***

2-7 September 2012, Skukuza, Kruger National Park (South Africa)

Number of Participants: Limited to 120 by the organizers

Level of involvement of SIG in the activity:

O ECA Individual Members registered with the SIG involved in the organizing committee: Leonard J. Barbour (Chairman), Susan Bourne, Mino Caira, Catharine Esterhuysen, Delia Haynes, Tanya le Roex, Luigi Nassimbeni, Clive Oliver, Melanie Rademeyer, Dave Billing, Lee Brammer, Ashwini Nangia, Karl W Törnroos.

O ECA Individual Members registered with the SIG involved as lecturers: Christer Aakeröy, Dave Billing, Jan Boeyens, Lee Brammer, Graeme Day, Claude Lecomte, Andreas Roodt, Jonathan Steed, Dyanne Cruickshank, Kinga Suwinska, Andreas Lemmerer, Petra Bombicz, Manuel Fernandes, Susan Bourne, Alessia Bacchi.

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

Sponsored by ECA? No

Other Sponsors/Organizers: IUCr, Bruker, CCDC, RSC, South African Crystallographic Society.

Short Description:

The last Indaba, dedicated to the theme "Insights from Structure", was the seventh in this series of interdisciplinary workshops considering various aspects of molecular structure (crystallography, spectroscopy, theory, etc.) and directed at all molecular scientists from chemistry, biology, physics, materials science and related fields.

MIRSIG was well represented at the Indaba 7. Many of the organizers are members of MIRSIG, and the programme showed their influence. Moreover, we are very glad to announce that during the Indaba 7, the Jan Boeyens Award has been assigned to our member Manuel Fernandes.

## 9. Future/Programmed Activities.

**Year 2013:** During the last months of 2012 and the winter 2013 MIRSIG has contributed to the definition of the scientific programme of ECM28 with a proposal based on the many suggestions received from our members. Only a part of this proposal was actually accepted, with great disappointment of many MIRSIG members who did not appreciate the reduced space assigned to our SIG.

At the **ECM28** (Warwich, 25-29 August 2013) MIRSIG has promoted:

one Keynote Lecture:

- PL1. Susan Bourne: "Building responsive metal-organic frameworks: modifying properties by structure"

and four Microsymposia, out of which one in collaboration with GIG #1 and three in collaboration with SIG #13.

- MS23 - Exploring crystal energy landscapes and crystal structure prediction (Chair: Graeme Day - Co-chair: Andrew Maloney) (with GIG1-YC)
- MS24 - Organic and inorganic multi-component crystals: structure and properties (Chair: Niki Bathori - Co-chair: Andrew Bond) (with SIG 13)
- MS25 - Molecular interactions: hydrogen bonding, halogen bonding, and beyond (Chair: Paola Gilli - Co-chair: Kari Rissanen) (with SIG 13)
- MS38 - Molecular recognition and complexation in small molecules (with SIG 13) (Chair: Alessia Bacchi - Co-chair: Janusz Lipkowski)

We would like to remark that four microsymposia joint with another SIG correspond to a total of only two MIRSIG microsymposia, which is pretty far from the numbers usually granted to our SIG during the last ten years as well as from our original proposal, which consisted of nine microsymposia, out of which six in collaboration (total of six).

Though some reduction of our requests could be expected, in view of the concurrent crystallographic centenary celebrations, we are surprised for the present considerable reduction,

which cannot certainly be imputed to the scientific MIRSIG level or to the too low attendance of our microsymbosia from our foundation.

We hope that the reason has to be identified in a number of practical difficulties in the organization of the meeting, and that in future ECMs the number of MIRSIG microsymbosia will come back to the average value of six registered so far.

We also hope that in the future the decisions of the Focus Area representatives will come back to the Programme Committee to be discussed with the SIG representatives before becoming operative, particularly when, as in the present case, significant changes of the SIG's proposals are involved.

To conclude with ECM28, it has to be noticed that our MIRSIG has been added as jointed SIG to other four MSa independently proposed by other SIGs and of interest for our members:

- MS10 - General interests of single molecule crystallography, both large and small  
(Chair: Thomas Schneider - Co-chair: Kirsten Christensen) (with SIG 1 and SIG 13)
- MS29 - Getting more from your electron density (with SIG 2 and SIG 9)  
(Chair: Claude Lecomte - Co-chair: Annamaria Mazzone)
- MS30 - Beyond harmonic treatment (with SIG 2 and SIG 9)  
(Chair: Birger Dittrich - Co-chair: Simon Grabowsky)
- MS39 - Crystallisation and crystal treatment (with GIG1, SIG 1 and SIG 13)  
(Chair: Terese Bergfors - Co-chair: Jose Gavira)

During the **year 2014**, because of the concomitant *XXIII Congress and General Assembly of the IUCr* (Montreal, 5-12 August 2014), the activity of MIRSIG will be reduced, since no specific MIR commission has been established in the IUCr, but not suspended, because several MIRSIG members (Enrique Gutierrez-Puebla, Dave Billing, Paul Raithby, Jim Wuest, our past-chairman Susan Bourne and the IUCr president Gautam Desiraju) are involved in the organization of this congress, which represents the main international event for the crystallographic community.

As for the **year 2015**, the MIRSIG activities will certainly include the *ECM29* (Rovinj, 23-28 August 2015). MIRSIG is preparing a number of suggestions for microsymbosia and plenary lectures to be held at ECM29. All MIRSIG members are kindly invited to give their active contribution to the scientific programme of the next ECM suggesting names of speakers and titles of microsymbosia by e-mail to the Secretary or, better, during the **2013 MIRSIG Assembly** that will be held in occasion of ECM28, and is scheduled for **Monday 26 August, 14:00–15:00, Arts Centre Cinema** of the Warwick University.

## **10. Other matters. ---**

### **11. Brief annual activity report**

During the period 2012-2013 SIG 7 has been actively involved in its prime purpose – to organize discussions, sessions and microsymbosia 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 recognizes the need for a SIG 7 mailing list and website which could act as a permanent point of contact among MIRSIG members, 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 ECM27 (Bergen) in August 2012:

Chairman: Carl Henrik Görbitz (University of Oslo) <c.h.gorbitz@kjemi.uio.no>

Co-Chairman: Graeme Day (University of Southampton) <G.M.Day@soton.ac.uk>

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