

**SIG: SIG # 7: MOLECULAR INTERACTION AND RECOGNITION
SPECIAL INTEREST GROUP (MIRSIG)**

Reported Period: 2008-2009

Report Date: 31 May 2009

Reported by: Paola Gilli (Secretary)

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1. Introduction.

The present MIRSIG Board, elected for the next three years by the Assembly of MIRSIG members, held on 8 August 2006 in Leuven during ECM23, is expiring at the end of August 2009 after the normal three-years period.

Chairman: Roland Boese (Essen) <roland.boese@uni-due.de>

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

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

A new MIRSIG Board has to be elected during the next Assembly of MIRSIG members, to be held in Istanbul during ECM25, in a date and place that will be communicated to all members in the near future, together with the candidatures for the years 2009-2012.

2. Past Activities.

Report on MIRSIG activity in 2008. During the year 2008, because of the concomitant XXI Congress and General Assembly of the IUCr (Osaka, Japan, 23-31 August 2008), the activity of MIRSIG has been reduced but not suspended. Though the SIG was not officially involved in the definition of the programme, many MIRSIG members have contributed to the success of the Osaka IUCr Congress as appointed chairs, co-chairs and invited speakers.

Report on MIRSIG activity in 2009 (Part 1/2).

ISIC-12: XII International Seminar on Inclusion Compounds (Stellenbosch, South Africa, 4-9 April 2009).

Number of Participants: 80

Sponsors: Bruker AXS, University of Stellenbosch, Cape Peninsula University of Technology, The National Research Foundation

Organizers: Prof. Len Barbour, Chairperson (Stellenbosch)

Prof. Susan Bourne (UCT); Prof. Mino Caira (UCT); Dr Liliana Dobrzańska (Stellenbosch); Dr Tanya le Roex (Stellenbosch); Prof. Luigi Nassimbeni (UCT & CPUT); Dr Clive Oliver (UCT); Dr Leslie Petrik (UWC); Dr Gaelle Ramon (CPUT)

Report: 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 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. The 12th edition, ISIC-12, was hosted on the campus of Stellenbosch University from April 4 to 9, 2009. The Organizing Committee, chaired by Len Barbour, was composed of MIRSIG members and, accordingly, our SIG was well represented among the participants. The conference featured a stimulating scientific programme encompassing all aspects of chemistry, mainly focussed on inclusion

phenomena in supramolecular chemistry, life sciences, nanotechnology and advanced materials.

3. Future/Programmed Activities.

Report on MIRSIG activity in 2009(Part 2/2). During the last months of 2008 and the winter 2009 MIRSIG has contributed to the definition of the scientific programme of ECM25 with the organization of two plenary lectures and five microsymbiosia, out of which one in collaboration with SIG 1 (Macromolecular Crystallography).

At the *ECM25* (Istanbul, 16-21 August 2009) MIRSIG has promoted:

two Plenary Lectures:

- PL1. Piero Ugliengo : "Modelling of biomaterials: molecular recognition at the surfaces of bioactive glasses"
- PL2. Christer B. Aakeroy: "Engineering co-crystals using molecular sense and supramolecular sensibility"

and five Microsymbiosia:

- FA1-MS7 - Molecular recognition and drug design (with SIG 1)
(Chair: Wolfram Saenger - Co-chair: Richard Pauptit)
- FA4-MS2 - Design and properties of functional molecular materials
(Chair: Jürg Hulliger - Co-chair: Giuseppe Resnati)
- FA4-MS3 - Multicomponent crystals
(Chair: Kinga Suwinska - Co-chair: Andrew D. Bond)
- FA4-MS4 - Supramolecular architectures: from structure to function
(Chair: Leonard J. Barbour - Co-chair: Matyas Czugler)
- FA4-MS11 - Crystal energy landscapes: computation and uses
(Chair: Sarah L. Price - Co-chair: Martin U. Schmidt)

We take the occasion to thank the Chairperson of ECM25, Prof. Engin Kendi, and the Program Committee for the space granted to MIRSIG subjects within this meeting.

Other activities 2009. One of the major aims of MIRSIG is always been that of establishing new relationships and maintaining old ones with scientific associations that pursue MIR studies outside the ECA, following the general policy of diffusion of the structural and crystallographic thought among other scientific disciplines. In addition to the already reported participation to ISIC-12, during the year 2009 several MIRSIG members have contributed (as members of the Organizing and/or Program Committee, and /or of the International Advisory Board) to the organization of the two following meetings, that will certainly be attended by a consistent number of MIRSIG members and on which we will report in detail next year.

INDABA VI: Structure and Properties (Berg-en-Dal, Kruger National Park, South Africa; 30 August - 4 September 2009)

Sponsors: IUCr (Structural Chemistry Commission); Bruker

Organizers: South African Crystallographic Society

Indaba 6 considers fundamental understanding of molecular science: structure, dynamics, activity and function. Molecular scientists from chemistry, biology, physics and materials science will contribute.

XVIII International Conference on “Horizons in Hydrogen Bond Research” (Paris, France; 14-18 September 2009)

Sponsors: CEA, CNRS, DFG, ENS, UPMC

Organizers: Laboratoire Léon Brillouin

This interdisciplinary conference, organized every two years, reports all most recent advancements in H-bond studies dealing with structure, dynamics and function of molecular and supramolecular H-bonded systems (from isolated molecules to biomacromolecules and materials) in all fields of physical chemistry (spectroscopic and diffraction techniques and theoretical chemistry).

4. Other matters.

ECM26 (Darmstadt, August 2010). MIRSIG is preparing a number of suggestions for microsymbiosia and plenary lectures to be held at ECM26. All MIRSIG members will be invited by e-mail to the MIRSIG Assembly to give their active contribution to the scientific programme of the next ECM.

Elections of the new MIRSIG Board 2009-2012. As already reported in the introduction, according to the SIG's rules a new MIRSIG Board has to be elected during the next Assembly of MIRSIG members, to be held in Istanbul during ECM25.

5. Five year ‘overview’, brief activity report (2005-2009)

MIRSIG was established in 1999 with the aim of promoting the inclusion of MIR activities in workshops and meetings, with particular regard to ECA annual meetings, and the cooperation with other scientific associations in the field of crystallography and physical and structural chemistry of molecular interactions. It has now some 180 members covering the complete spectrum of theoretical, general and applicative fields of MIR. Since 2005 MIRSIG has collaborated with other associations to the organization of six workshops and conferences and contributed to the scientific programme of ECMs with 1-2 plenary lectures and 5-6 microsymbiosia *per* meeting, all events attended by a wide audience testifying the interest of the European crystallographic community for MIR studies.

Because of its interdisciplinary nature, MIRSIG has organized over the years several joint microsymbiosia with other SIGs and, in particular, a consolidated collaboration with SIG#1 (Macromolecular Crystallography), SIG#2 (Charge, Spin and Momentum Densities) and SIG#13 (Molecular Structure and Chemical Properties) has been established. Notwithstanding we have to remark that, mostly because of the long and complex procedure of definition of the ECM scientific programme, the organization of joint activities is always cumbersome and may sometimes become impossible. Of course any effort will be made by MIRSIG to overcome these difficulties in the future.

6. Estimated number of active members: 180

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

Chairman: Roland Boese (Essen) <roland.boese@uni-due.de>

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

Supplementary Materials. None.

Report compiled by:

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