

## **SIG13**

**Reported Period: June 2016 –June 2017**

**Report Date:**

**Reported by: Alessandra Crispini (SIG Chair)**

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

During the last year the SIG13 committee has reinforced both the reorganisation and promotion of the SIG to the structural science community, participating actively in the scientific organization of the 31st European Crystallographic Meeting, ECM31, will take place in Oviedo, Asturias, Spain from 22-27 August 2018. SIG13 representatives have been active in the development of the programme for the ECM31 meeting and have made major contributions to the setting up, in strong collaboration with other SIGs (SIG 7 and 11). In particular, Dr. Clive Oliver has strongly contributed to the development of the ECM31 scientific program within the SIG13 community. All SIG13 members have been involved actively in the organization of events and meeting devoted to the diffusion of structural studies within the field of materials properties.

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

SIG13 <http://ecanews.org/mwp/groups/sig-13-molecular-structure-and-chemical-properties/>

### **3. Number of SIG-13 members according to** (<http://ecanews.org/mwp/groups/sig-13-molecular-structure-and-chemical-properties/>)

SIG13 Molecular Structure and Chemical Properties            199

### **4. Existence of a SIG mailing list: Yes**

**Address of the mailing list:** Mailing list through ECA website

**Number of members in the SIG mailing list:** 199

Through the ECA website above as well as the ECA-SIG13 facebook home page it is possible to advertise all events related to our activities: <http://www.facebook.com/pages/ECA-SIG13/137466489407>.

**5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)** 199 from ECA website but additional contacts through French, British, Italian, Spanish and South African Crystallographic Associations.

### **6. List of MS proposed by the SIG-13 (also in collaboration with other SIGs) at the ECM31**

<b>Microsymposium topic/title</b>	<b>SIG / SIG</b>
1. Molecular Structure and Chemical Properties: Chemistry meets Charge Density	SIG 2 / SIG 13
2. Electron crystallography methods for structure characterization of small molecule organic and hybrid materials	SIG 4 / SIG 13

<b>Microsymposium topic/title</b>	<b>SIG / SIG</b>
3. From 0- to 3-dimensional organic porous systems	SIG 13
4. Simulations of molecular crystals	SIG 13 / SIG 7
5. Exploring the structure by NMR crystallography	SIG 13
6. Non-stoichiometric systems: solid solutions or mixed crystals	SIG 13
7. Structure and function in inorganic and coordination compounds	SIG13
8. Mechanochemistry: structure and reaction	SIG 13
9. Photochemistry: optical properties of crystals	SIG 13
10. Halogen bonding in the solid state	SIG 7 / SIG 13
11. The role of supramolecular interactions in polymorphs and co-crystals	SIG 7 / SIG 13
12. Molecular recognition and crystal engineering	SIG 7 / SIG 13
13. Lattice energy calculations as a tool to understanding structure	SIG 13 / SIG 7

**Prizes sponsored/coordinated**

none

**8. Past Activities other than Microsymposia at ECM**

Title: 23<sup>rd</sup> International Conference on the Chemistry of the Organic Solid State

Number of Participants: 100

Level of involvement of SIG in the activity: Several ECA members were part of the organizing committee, which was chaired by Len Barbour.

Sponsored by ECA: no

Other Sponsors/Organizers: none

Short Description: This conference is part of an international series held around the world. All aspects of the chemistry and physics of organic materials are included in the scope of the conference. The website: [icross2017.co.za](http://icross2017.co.za)

Title: BCA Spring Meeting, 4-7 April, 2016, University of Nottingham (included here because not in the 2016 report)

Number of Participants: 150

Level of involvement of SIG in the activity: Several ECA members are part of the organizing committee.

Sponsored by ECA: no

Other Sponsors/Organizers: CCDC, Bruker, Panalytical, Rigaku.

Short Description: With the 2<sup>nd</sup> century of X-ray diffraction now well underway, the BCA 2016 Spring Meeting programme has taken stock of the current state-of-the-art and continue to look towards the future.

Title: 10th Edition of Symposium with International Participation: New Trends and Strategies in the Chemistry of Advanced Materials with relevance in Biological Systems, Techniques and Enviromental Protection, Institute of Chemistry, Timisoara (Romania), 08-09 June 2017.

Level of involvement of SIG in the activity: ECA members participants

Number of participants: 60

Sponsored by ECA: no

Other Sponsors/Organizers: none

Short Description: The main goal pof the Symposium is to present the latest trends in the chemistry of materials, with reference to theor structures and therefore new applications.

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**SIG-13 also provided support letters to Tony Linden (Zurich School of Crystallography: 11-22 June 2017) and Anton Meden (Slovenian Croatian Crystallographic Meeting 2017: 15-17 June and in aid of ECA sponsorship applications.**

## **9. Future/Programmed Activities.**

Title: 1<sup>th</sup> International Symposium on Metallacrowns and Metallacryptates, which will be held in Parma on the 27-28 of September 2017

Number of Participants: 100

Level of involvement of SIG in the activity: ECA members are part of the organizing committee.

Sponsored by ECA: to be applied for

Other Sponsors/Organizers: to be applied for

Short Description: The Symposium is held as the final meeting of the EUFP7 Marie Curie IRSES Project “Metallacrowns” and as the final meeting of the Bilateral Italy.USA Project “Development of porous magnetic Metallacrowns for sensing applications”. Within the Marie Curie Project, Dr Matteo Tegoni and the involved team of the Department of Chemistry, Life Science, and Environmental Sustainability of the University of Parma, have been strongly involved in the work package of title “X Ray Structures of large MC Assemblies”, designing, synthesizing and structural characterizing (X ray) large MC assemblies including MOF-like architectures.

**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) by participating effectively in the planning process for the upcoming ECM and other Meetings in Crystallography.

A SIG-13 meeting was held during ECM30 in Basel on 31 August 2016. The SIG officers presented the 2016 report to the meeting. The members discussed cooperation between SIG-13 members and the possibility of a triennial scientific meeting around specific themes. An immediate outcome of the meeting was the nomination of Clive Oliver to the ECM-31 Programme Committee as the SIG-13 representative. Updating of the SIG-13 website in terms of adding content to the “Scope and Objectives” section, to include more activities and thus improving visibility and publicity of SIG-13 Clive Oliver mentioned that the new website is intended to be used for the dissemination of information to SIG-13 members (the meeting notice was also sent via the website), thus negating the need to have a continually updated e-mail list.

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

\* *Chair:* Prof. Alessandra Crispini (responsible for the general coordination of the SIG, and specially for interacting with the steering committee)

*E-mail:* crispini@unical.it

*Address:* MAT-INLAB (Laboratorio di Materiali Molecolari Inorganici), Structural Chemistry Section  
Department of Chemistry and Chemical Technologies  
Cubo 14C, Via P. Bucci  
University of Calabria (UNICAL)  
87030 Arcavacata di Rende (CS), Italy  
(Tel: +39 0984 492888 Fax: +39 0984 492067)

\* *Co-chair:* Prof. Petra Bombicz (responsible for coordination of the SIG activities and for implementing/distributing news of SIG interest)

*E-mail:* bombicz.petra@ttk.mta.hu

*Address:* Research Group of Chemical Crystallography, Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Magyar Tudósok körútja 2, H-1117 Budapest, Hungary

Tel: +36 1 382 6513

\* *Secretary:* Dr Clive Oliver (responsible for the SIG web-page and for maintaining the SIG13 mailing list)

*E-mail:* [clive.oliver@uct.ac.za](mailto:clive.oliver@uct.ac.za)

*Address:* Centre for Supramolecular Chemistry Research, Department of Chemistry,  
University of Cape Town, Rondebosch, 7701, South Africa  
Tel: +27 216503830; Fax: +27 216505195