Commission on Inorganic and Mineral Structures (CIMS) of the IUCr

Report for the Year 2014

Members and consultants of CIMS discussed various issues via email. Other forms of communication were given by occasional other meetings or conferences (in particular, a meeting was held in Montreal during the IUCr congress), or by using the website. The latter is kindly maintained by M. Nespolo (http://www.crystallography.fr/cims/).

The Commission on Structural Crystallography, CSC, of IUCr and CIMS maintained their links. P. Mercier is now the liaison person representing CSC in CIMS and vice versa.

P. Mercier continues to act as liaison officer of CIMS with IUCr Newsletter.

D. Pandey and F. Paz were appointed co-editors of, respectively, *Journal of Applied Crystallography* and *Acta Crystallographica Section C* on the recommendations of CIMS.

Strong links exist between CIMS and the European Crystallographic Association: O. Yakubovich (CIMS member) is member of the executive committee; the secretary of the Special Interest Group 5SIG5 is O. Siidra, the Chairman S. Krivovichev (CIMS consultant) and F. Hatert Vice-Chairman (CIMS member) (ECA-SIG5, http://sig5.ecanews.org/).

There are very good relationships between CIMS and the European Mineralogical Union (EMU, http://eurominunion.org/); R. Oberti (EMU past president) is member of CIMS and also Commissioning editor of the EMU Notes in Mineralogy. In 2014, EMU has organised the school "Planetary Mineralogy" (Glasgow, 25/8-3/9, main organisers M. Lee and H. Leroux), which was supported by an Erasmus Intensive Programme grant. The accompanying book of the EMU Notes in Mineralogy, vol. 15, will be published shortly. Volume 16 "Mineralogical crystallography", co-edited by J. Majzlan, Sergey Krivovichev (CIMS consultant) and J. Plasil, is presently under production.

CIMS also collaborates with the Geochemical Society and the European Association of Geochemistry: R. Oberti was co-editor of the special issue of the Mineralogical Magazine focused on the contribution to the session "GEOLIFE-Geomaterials for environment, technology and human activities" convened during the 2013 Goldschmidt Conference.

Changes of CIMS Members and Consultants

Several members came to end of office and the opportunity was taken to welcome new members and consultants:

Members Terminating Office – D. Pandy (India), P. A. Thomas (UK), T. Nagai (Japan);
Consultants Terminating Office – A. Thalal (Marocco), S.-L. Wang (Taiwan) W. Depmeier (now CIMS supervising member of IUCr EC);
New Members – Peter Burns (US), Marek Wołczyr (Poland), Akira Yoshiasa (Japan);
New Consultants – K. Byrappa (India), Raúl Carbonio (Argentina), Chris Ling (Australia), Dhananjai Pandey (India), Isabella Pignatelli (USA), Mark Welch (UK);

Member Patrick Mercier was nominated CIMS secretary.

**CIMS was involved in the following meetings held in 2014:**

- The main activity of CIMS in 2014 was the preparation and running of the following events at the 2014 IUCr Montreal congress: microsymposia (i) MS 1, chairs P. Thomas and K. Sugiyama, “Phase transitions in functional inorganic materials and minerals”; (ii) MS 15, chairs O. Yakubovich and S. Pereira, “The role of defects in crystal structure formation, organization and stability”; (iii) MS74, chairs P. Mercier and R. Peterson, “Mineralogical crystallography”. Moreover, D. Pandey delivered a keynote entitled: “The world of perovskites: phase transitions and exotic properties”.

- R. Oberti co-chaired the organizing committee of the first European Crystallographic School (ECS) held in Pavia 26/8-6/9 to celebrate the International Year of Crystallography. Some 120 students from 30 countries (selected from among 200 applications) and more than 20 internationally renowned teachers (including the Nobel laureate V. Ramakrishnan) contributed to the success of a 10-day school for master’s and PhD students and a 6-day school designed for students with expertise. The school was supported by an Erasmus Intensive Programme grant to a consortium of 9 European universities and provided students with 3 ECTS credits. The successful request of sponsorship to IUCr has been supported by CIMS.

- M. Nespolo and S. Krivovichev represented CIMS in the International Advisory Board of the 2014 Meeting of the International Mineralogical Association, held on 1-5 September 2014 in Gauteng, South Africa, where CIMS was in charge of the session "Modular Aspects of Mineral Structures" in the theme "Mineralogical Crystallography".

- J. Rocha was member of the organising committee of conference SMARTER4, held on 1-4 September 2014 in Durham University, UK (http://www.ccpnc.ac.uk/smaerter4/).

- Joint IUCr MaThCryst - CIMS Workshop: D. Pandey was workshop coordinator, M. Nespolo and J. Rocha were members of the international programme committee of the Workshop on “Symmetry relationships between crystal structures with application to structural phase transitions”, held in Varanasi, India, on 27-31 October, 2014 ((Dhananjai Pandey, Massimo Nespolo, Mois Aroyo and Juan Carvazal were lecturers). http://iitbhu.ac.in/conferences/mst/IUCr/).

- G. Ferraris and R. Oberti were members of the scientific committees for the organisation of two meetings celebrating IYCr in Italy: (1) "Impact of crystallography on modern science", was organized by the Accademia delle Scienze di Torino and held in Torino on June 25, 2014; a talk was given by Robert Hubert, Nobel laureate 1988, "Beauty and fitness for purpose, the architecture of proteins, the building blocks of life". R. Oberti talked on the impact of crystallography and crystal-chemistry on petrology and geochemistry. (2) "Challenges in Crystallography", was organized by the Accademia Nazionale dei Lincei, and held in Rome on October 13-14, 2014. CIMS chairman, J. Rocha, gave an invited talk.

- O. Yakubovich was member of the Organizing Committee of the XVIII International conference “Crystal chemistry, X-ray diffraction and spectroscopic studies of minerals”, held in Ekaterinburg, Russia, 2014.
CIMS has been involved in the organization of the following meetings:

- R. Oberti is member of the scientific committee of the 8th European Conference on Mineralogy and Spectroscopy to be held in Rome, 9-11 September 2015 (http://www.ecms2015.eu/). This event will deal with mineralogy, spectroscopy and related fields, with a special focus on the interplay between short-range and long-range information to account for crystalline and amorphous material’s physical properties.

- S. Krivovichev and R. Oberti are members of the scientific committee of the 2nd European Mineralogical Conference to be held in Rimini, 11-15 September 2016 (http://emc2016.socminpet.it/). The focus will be on the impact of crystallography on the mineralogy and petrology of the Earth and extraterrestrial bodies.


- O. Yakubovich is member of the Program Committee of the 29th European Crystallographic Meeting, to be held in Rovinj, Croatia on August 2015.

CIMS supported the application for funding by IUCr of the following meetings to be held in 2015:

- 8th USPEX Workshop, “Computational Materials Discovery Using the USPEX Code”, to be held at Shiv Nadar University, India, on 20-24 January 2005, promoted by Artem O. Oganov; D. Pandey gave the opening lecture.

- 8th European Conference on Mineralogy and Spectroscopy, to be held in Rome on 9 September 2015, promoted by R. Oberti (scientific committee).

24 March 2015.

Prof. João Rocha
(Chair of CIMS)