Report of the Commission on Mineral and Inorganic Structures (CIMS) for the year ending 31 December 2007

Contacts among the Members and Consultants of CIMS have been maintained mainly via e-mail and the web site http://www.crystallography.fr/cims/ administered by the consultant member Massimo Nespolo. Some members had the opportunity of meeting and discussing CIMS activity in occasion of the ECM 24 (Marrakech, Morocco, 20-27 August 2007).

CIMS has sponsored the application for financial support to IUCr of the following meetings that have been organized during 2007; the active participation of members of CIMS is given for each meeting.

1. XVI International Conference on crystal chemistry and diffractions studies of minerals (Miass, Russia, 2-6 July 2007 http://meetings.mineralogy.ru/Default.asp). W. Depmeier, G. Ferraris and D. Pushcharovsky were members of the Programme Committee; WD and GF were also invited speakers.
2. Workshop "Minerals as advanced materials" (Apatity, Russia, 8-12 July 2007). W. Depmeier and G. Ferraris were invited speakers. An outcome of this workshop is the volume "Minerals as advanced materials I" (S. V. Krivovichev editor) published by Springer.
3. International School on Mathematical and Theoretical Crystallography (Havana, Cuba, 15-20 July 2007; http://www.crystallography.fr/mathcryst/havana2007.htm). G. Ferraris and M. Nespolo were organizers and speakers of the school. The texts of the lectures are available on the site shown above.
4. ACA Annual Meeting (Salt Lake City, USA, 21-26 July 2007).
5. 41st IUPAC World Chemistry Congress (Torino, Italy, 5-11 August 2007 http://www.iupac2007.org/) to run the section 4a-4 "Structural aspects of crystalline materials (from inorganic to macromolecular)"; G. Ferraris was a proponent.
6. ECM-24 (Marrakech, Morocco, 22-27 August 2007) and its satellite conference "The enchanting crystallography of Moroccan ornaments" (Marrakech, Morocco, 20-22 August 2007). The satellite (http://www.crystallography.fr/mathcryst/marrakech2007.htm) has been organized by the IUCr MaThCryst Commission chaired by M. Nespolo, consultant member of CIMS. At ECM-24 P. Thomas and W. Depmeier were in the Programme Committee; J. Rocha was a keynote speaker; G. Ferraris and P. Thomas were chair of MS.
7. II International Conference "Crystallogenesis and mineralogy" (St. Petersburg, Russia, 1-5 October 2007 http://www.minsoc.ru/confs.php?cid=39) and its satellite "Structural chemistry of inorganic actinide and lanthanide compounds" (St. Petersburg, Russia, September 29 - October 1st, 2007). W. Depmeier was chair and invited speaker in both meetings. G. Ferraris and D. Pushcharovsky were members of the International Committee.
8. "Workshop on structure elucidation by combining magnetic resonance, computation, modelling and diffractions (SMARTER)" (Aveiro, Portugal, 6-7 September 2007, http://www.primarius.org/smarter/) organized by J. Rocha on behalf of CIMS; G. Ferraris was member of the International Committee. The aim of the SMARTER meeting was to bring together specialists from the different areas of materials science, such as materials chemists and processing engineers, diffraction and spectroscopy scientists, and computational structuralists, that may contribute to the development of a common language for a SMARTER approach to structure solving, using geometrical, diffraction, modeling and NMR crystallographic methods. SMARTER was attended by some 110 researchers, Ph.D students and post-docs from France, Germany, India, Italy, Poland, Portugal, Spain, UK and USA. The scientific programme consisted of 20 talks (most) 30' long and 12 posters. In a lively discussion at the end, the conferees found the SMARTER workshop concept very interesting and timely, and agreed that it would be useful to continue it and hold in 2009, in Aveiro, the second such event.
9. MSA-GS-ANL short course on "Amphiboles" (Rome, Italy, 29-31 October 2007,

http://www_crystal.unipv.it/amphiboles/home.htm). F. C. Hawthorne, consultant member of CIMS, was an organizer and speaker. An outcome of this short course has been the volume "Amphiboles: Crystal Chemistry, Occurrence, and Health Issues" (F.C. Hawthorne, R. Oberti, G. Della Ventura, A. Mottana editors), No. 67 of the series "Reviews in Mineralogy and Geochemistry".

10. CIMS contributed to suggest topics and authors for the special issue "60 years of *Acta Crystallographica* and the IUCr"; D. Pandey co-authored the article "Stability of ferroic phases in the highly piezoelectric $Pb(Zr_xTi_{1-x})O_3$ ceramics".

During 2007 CIMS has been active for the organization of the following meetings to be hold in 2008.

1. II International Workshop on Layered Materials "Structure and Properties" (Vercelli, Italy, 28-29 March 2008 http://www.layeredmaterials.mfn.unipmn.it/). G. Ferraris is member of the Organizing Committee. W. Depmeier, G. Ferraris and D. Pandey are members of the Programme Committee. J. Rocha is an invited speaker. As SMARTER in 2007, this workshop intends to attract researchers, like materials scientists, who, in spite of their high-level crystallographic production, are not regular attendees of IUCr general meetings.
2. Pam Thomas represented CIMS in the Programme Committee of IUCr XX1 (Osaka, Japan, 23-31 August 2008); taking into account suggestions from CIMS members, she was able to include the following events of specific interest for our Commission (some of them are shared with other IUCr Commissions). (1) MS70 "Crystal chemistry and crystallography of aperiodic crystals"; (2) MS77 "Diffuse scattering in partially ordered/disordered systems; (3) MS93 " Crystallography of planetary materials at extreme conditions"; (4) MS94 "From minerals to materials"; (5) MS95 "Multitechnique approach to the determination of inorganic structures"; (6) MS97 "Perovskites and related materials"; (7) MS98 "Structure-properties correlations and phase transition in inorganics"; (8) KN11 "Crystallochemical basis of synthetic mineral immobilizations", speaker T. White; (9) KN36 "Structure refinement and structure modelling: a chemical probe for complex mineral groups", speaker R. Oberti; (10) KN23 "Structural phase transitions", speaker J.M. Perez-Mato; (11) G. Ferraris, M. Nespolo and D. Pandey will be chair of MS or KN sessions.

Besides the activity given above, members of CIMS have reported to the Chair the following personal activity related to the purposes of the Commission.

W. Depmeier - Keynote lecture at the Jahrestagung "Deutsche Gesellschaft für Kristallographie", Bremen, Germany, 5. - 9. 3. 2007; invited speaker at workshop on "Time- and temperature-resolved X-ray powder diffractometry: New developments in technique and applications", Fraunhofer ICT, Berghausen, 8. -9, November 2007; Chairman of SIG 5 "Mineralogical Crystallography" of the European Crystallographic Association.

M. Matsui - Editor of Physics and Chemistry of Minerals.

L. McCusker - Invited lectures: Canadian Society for Chemistry Meeting, Winnipeg, Canada "Deciphering the structural information in a zeolite powder diffraction pattern"; Berzelii Centre EXSELENT on Porous Materials, University of Stockholm, Sweden "Zeolite structures and their determination from powder diffraction data"; Rayons X et Matière, RX2007, Dijon, France "Combining techniques to solve complex zeolite structures". Co-author (with Christian Baerlocher and David H. Olson) of the 6th revised edition of the *Atlas of Zeolite Framework Types* (Amsterdam, Elsevier). Member of the Program committee for IZC-15, Beijing, China. Co-editor for *Acta Crystallogr. B.* Maintenance of the IZA websites (*http://www.iza-online.org/* and *http://www.iza-structure.org/*); redesign (together with Christian Baerlocher) of the web Database of Zeolite Structures (*http://www.iza-structure/databases/*).

M. Nespolo - Associated editor of the European Journal of Mineralogy; secretary of the Special Interest Group SIG5 "Mineralogical Crystallography" of ECA.

D. Pandey - Microsymposium Chair for Functional Materials at the International Conference

on Advanced Materials (sponsored by IUMRS) held in Bangalore in 2007.

D. Pushcharovsky - Associate Editor of the European Journal of Mineralogy.

J, Rocha – Member of the editorial board of the European Journal of Inorganic Chemistry

E. Tillmanns: chief editor of the European Journal of Mineralogy; chair of the Organizing Committee of the 20th General Meeting of the International Mineralogical Association (IMA) (Budapest, Hungary, 2010).

Giovanni Ferraris, Chair