



**Schweizerische Gesellschaft für Kristallographie  
Société Suisse de Cristallographie  
Swiss Society for Crystallography**

**Sektion für Kristallwachstum und Kristalltechnologie  
Section de Croissance et Technologie des Cristaux**

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the Swiss Academy of Sciences



**SGK/SSCr NEWSLETTER**

**No. 70**

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Report on the EPDIC-10 Conference in Geneva

### **On the Cover:**

Two of the user facilities at PSI celebrate round birthdays: The 5<sup>th</sup> birthday of the start-up of the SLS user operation in 2006 (see report on page 7), followed by the 10<sup>th</sup> birthday of the neutron spallation source SINQ in 2007.  
(Foto: Courtesy of Paul Scherrer Institut, Villigen)

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## Letter from the President

**Walter Steurer (Walter.Steuer@mat.ethz.ch)**

The year 2006 was a good year for the Swiss Society of Crystallography (SSCr). Two of our members received prestigious awards, Prof. Tim Richmond and Dr. Artem Oganov, both from ETH Zurich. Please, forgive my ignorance if I am not aware of other prizes which may have been awarded to some of our members. Tim Richmond received the Marcel Benoist Prize (CHF 100'000) for his impressive work on the structure of the nucleosome, a complex of DNA and proteins that constitutes the sub-unit from which the chromosomes of living cells are built. Artem Oganov's work was rewarded with the ETH Zurich Latsis Prize (CHF 25'000) for his exciting contributions to computational crystallography such as the discovery of the post-perovskite which is located at the mantle-core boundary region of the Earth and his recent achievements in crystal structure prediction.

The year 2006 has also seen the retirement of some of our most active members. I just want to mention three of them, Prof. Hans-Beat Bürgi, University of Berne, Dr. Hans Grimmer, PSI, president of the SSCr from 2000 to 2002, and Dr. Volker Gramlich, ETH Zurich, member of the SSCr committee for many years. We also moan the death of Prof. Erwin Parthé (1928-2006) and Prof. Johann Jakob Burckhardt (1892-2006). For their obituaries see pages 34 and 33, respectively.

In the year 2006, however, the SSCr also welcomed many new members keeping the number of active members more or less constant. Fortunately, the statistics on the age distribution of our members (see page 36) shows two peaks. One is centered around age 55, the other at age 35.

Recently, I stumbled across an interesting bibliometric study in crystallography (Behrens & Luksch, Acta Cryst. B62, 2006, 993) concerning the Inorganic Crystal Structure Database. The number of entries per year into this database can be described by a simple quadratic function. It increased from about 250 entries in 1950 to 3500 in 2000 and will reach 4300 in 2010, 5500 in 2020 and 6800 in 2030. Remarkably, this curve does not show any discontinuity marking the advent of area detectors in the nineties of the last century. Obviously, for 'small crystal structures', CCD detectors did not have much impact on the throughput. On the other hand, the community of authors is growing just linearly by 203 authors per year. Taking into account the exponential increase of the average number of coauthors of a paper, from 1.4 in 1920 to 4.2 in 2004, we see a steady increase in productivity that should please the bean counters in our universities.

I wish you a pleasant and productive 2007.

Walter Steurer  
President of the SSCr



## **5 Years of SLS**

**by J. Friso van der Veen (friso.vanderveen@psi.ch)**

### **Facility**

The Swiss Light Source celebrates in 2006 five years of operation. Mid 2001 the materials science and protein crystallography beamlines saw the first light, and soon thereafter the beamlines for surface and interface spectroscopy and microscopy. The SLS now has some ten beamlines operating, and will have 18 to 20 beamlines in 2011. By then the SLS can be considered to be a fully-grown facility, certainly when taking into account the small size of Switzerland.

The SLS is a third-generation synchrotron radiation facility of medium electron energy (2.4 GeV), which produces high-intensity x-ray beams up to ca 18 keV by use of the higher harmonics of small-gap in-vacuum undulators. The setting of small undulator gaps (4-5 mm) is possible thanks to low beam emittance, combined with top-up injection of the electrons, which compensates for a possible decrease of lifetime of the stored electron beam. Since many x-ray diffraction studies are performed in the range up to 20 keV, a medium-energy machine such as the SLS is competitive with the high-energy ones in many areas of science, against a fraction of their costs. At a photon energy of 10 keV, medium-energy sources typically have an order of magnitude smaller brilliance than, e.g., the ESRF. In the soft x-ray range they are of course superior in performance. Top-up injection is essential for another important reason. A constant stored current in the ring gives rise to a constant heat load on the ring chamber including the electron optical elements along its circumference. This has made the SLS a world champion in beam stability. The (generally) happy user may find out that the (almost) 'impossible' experiment becomes possible. Just for the record, the SLS is a user facility open to scientists from Switzerland and abroad. Two laboratories within the SLS are responsible for the operation and construction of beamlines. One laboratory (C. Quitmann) covers materials science, solid-state spectroscopy and microscopy, the other one (R. Abela) all other disciplines, including detector development. The Laboratory for Micro- and Nanotechnology (J. Gobrecht), which also belongs to the department operating the SLS, is fully integrated into the activities at the SLS.

Access to the SLS is provided through the selection of proposals for beam time by an international review committee. The selection is solely based on scientific merit. Currently, about 40 % of the SLS users are from the EU countries. Beam time at the SLS is heavily in demand, and Swiss scientists compete for access with the strongest user groups worldwide. Access by users from the EU is facilitated by the Integrating Activity IA-SFS of the FP6 program of the EU. In addition to providing user support and constructing new beamlines, SLS staff members pursue research projects of their own. This is important for the local scientific culture and ensures user support of high quality. The SLS also provides services to industrial users. In 2005, ca 10% of the total beam time has been sold to companies (mostly pharmaceutical) for proprietary research. Companies are charged for proprietary work on the basis of full cost recovery.

## **Mission**

Our mission is to provide photon beams to researchers in the natural sciences. Our strategy is to excel in a number of selected disciplines rather than trying to serve the needs of *all* users. Major thrust areas are: structural biology, biomedical imaging, nanoscale magnetism, properties of correlated electron systems and pico- and femtosecond x-ray spectroscopy. Internationally well recognized are our R&D efforts in pixel detectors and x-ray optics. At one of the absorption spectroscopy beamlines, hard x-ray pulses of 50-100 fs duration are generated by use of the electron beam slicing method. This is the world's brightest source of femtosecond hard x-ray pulses (up to ca 20 keV) until the x-ray free electron lasers in Stanford and Hamburg start operation and take over. SLS fruitfully collaborates with external groups which bring new instruments or methods to the SLS or act as 'power users'. These groups contribute financially or in kind to the construction and running of beamlines (e.g., Uni Zürich, EPFL, NCCR Structural Biology, EMPA, Max-Planck-Gesellschaft (MPG), CNRS/SOLEIL, Politecnico Milano, Uni Erlangen).

Scientific output from the SLS in the years 2004, 2005 and 2006: in total ca 450 papers, of which 48 in top journals (Nature, Science, Cell, PRL). This output will increase with the number of beamlines in operation.

## **Science**

The research area currently having the highest impact is undeniably structural biology. In order to remain at the forefront, the SLS invests substantially in instrumentation and manpower. The beamlines for protein crystallography (PX-I and PX-II) are generally recognized as being the world's best in their kind. They attract internationally reputed structural biologists from academia as well as those from leading pharmaceutical companies. Roche, Novartis and MPG have jointly financed an entire beamline, including its operation. The biology groups from ETH, Uni Zürich and the BIO Department at PSI are all important users. The SLS invests in innovative pixel detectors for PX, facilities for diffraction from micrometer-sized protein crystals, robotics and web-based services such as mail-in crystallography. A spin-off firm in pixel detectors has recently been founded.

Solid-state spectroscopy is also one of our priority areas. The beamline for surface and interface spectroscopy offers full control over the polarization of the XUV radiation and has a station for angle-resolved photoemission spectroscopy (ARPES). Swiss users investigate, e.g., properties of correlated electron systems, including high  $T_c$  superconductors and oxides exhibiting colossal magnetoresistance. Competition worldwide is severe. The SLS now invests in an upgrade of the ARPES station so as to make it the world's most advanced beamline in its kind. An important new tool is the beamline 'ADRESS' for high-resolution resonant inelastic x-ray scattering (i.e., Raman spectroscopy with x rays), which starts operation in 2007. In addition, a facility for IR-spectroscopy will soon become available.

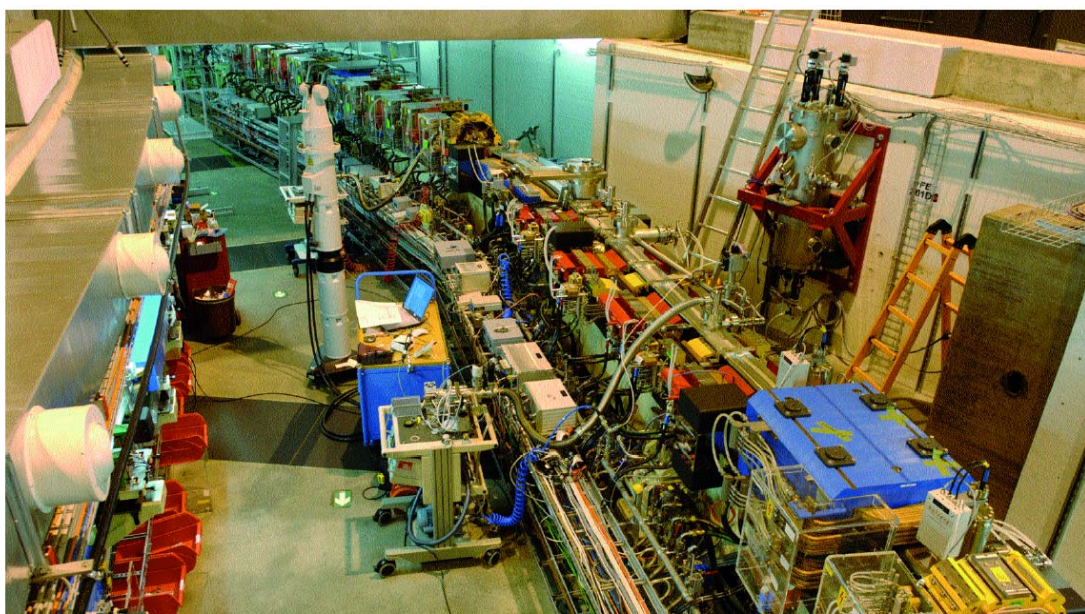
Another important topic is the dynamics of nanoscale magnetic systems on a picosecond time scale, for which the SLS offers a unique measurement platform. Orbital and spin ordering in metal-oxides are investigated using resonant soft x-ray scattering.

The beamline for materials science and tomography attracts a wide range of users. Unique is time-resolved (millisecond) powder diffraction using a strip detector developed in-house. The facility is complementary to that at the Swiss-Norwegian beamline at ESRF.

X-ray absorption spectroscopy (XAS) using a microfocus beam is much in demand by chemists and environmental scientists. The beamline 'LUCIA', operated jointly with CNRS/SOLEIL, offers unique facilities for  $\mu$ -XAS and x-ray fluorescence in the difficult photon energy range of 0.9 to 6 keV. It also attracts geophysicists studying condensed matter under high pressure. The beamline ' $\mu$ -XAS' is used for studies of radioactive samples and for pump-probe studies of the dynamics of molecules in solution (EPFL).

For the period 2008-2011, the following major thrust areas have been defined: (1) femtoscience with x-rays and (2) life sciences, in particular structural biology and bioimaging on all relevant length scales. As to the latter area, a third beamline for protein crystallography including a platform for on-site crystallization is under construction. Furthermore, a beamline for tomography and medical radiology will be dedicated to imaging on (sub-)micrometer and small-animal length scales (with EPFL). IR-microscopy is in development, as is a facility for solution scattering and coherent scattering at the beamline 'cSAXS'.

The SLS has a bright future for years to come!



View in the tunnel of the Swiss Light Source at Villigen/PSI, showing the magnets around the electron storage ring.

## La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub>, Containing Isolated [Ni<sub>2</sub>H<sub>7</sub>]<sup>7-</sup> and [Ni<sub>4</sub>H<sub>12</sub>]<sup>12-</sup> Anions

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Following our discovery of a hydrogen induced insulating state in the LaMg<sub>2</sub>Ni-H system [1] we have investigated the closely related La<sub>2</sub>MgNi<sub>2</sub>-H system. Hydrogenation of tetragonal La<sub>2</sub>MgNi<sub>2</sub> leads to a complex metal hydride of composition La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> having monoclinic symmetry. In contrast to LaMg<sub>2</sub>NiH<sub>7</sub> which displays mononuclear tetrahedral [NiH<sub>4</sub>]<sup>4-</sup> complexes that are isolated from each other, La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> [1] displays two types of polynuclear hydrido complexes having novel geometries, dinuclear [Ni<sub>2</sub>H<sub>7</sub>]<sup>7-</sup> and tetranuclear [Ni<sub>4</sub>H<sub>12</sub>]<sup>12-</sup>. The complexes are ordered and represent the first such case for a 3d system in the literature. The Ni-H distances vary from 1.50 to 1.71 Å. Some hydrogen atoms are coordinated by La and Mg atoms only in octahedral [La<sub>4</sub>Mg<sub>2</sub>]-type or tetrahedral [La<sub>2</sub>Mg<sub>2</sub>]-type configurations. The hydride does not desorb hydrogen below 200°C and 1·10<sup>-1</sup> mbar pressure and segregates into LaH<sub>3</sub> and other unidentified phases above 300°C. Electrical resistance measurements on powder samples confirm the hydride to be non-metallic.

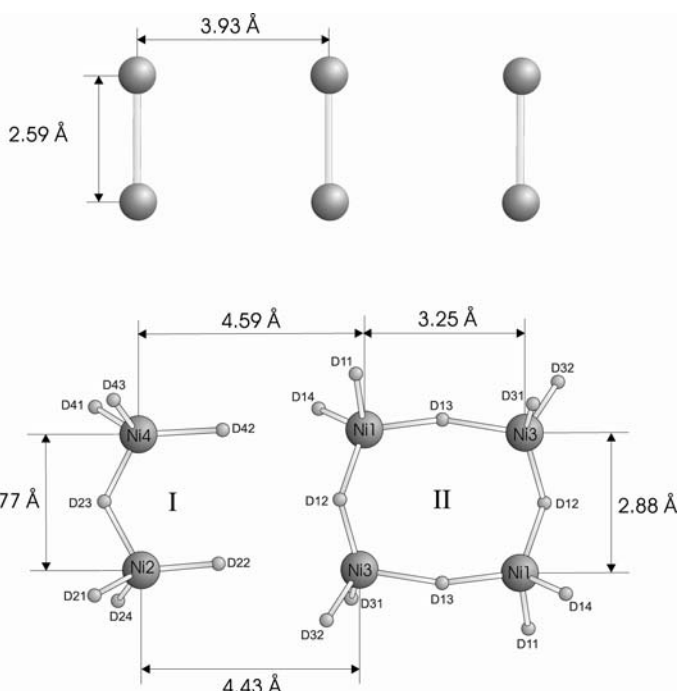
Title compound was obtained by direct hydrogenation of the intermetallic La<sub>2</sub>MgNi<sub>2</sub> [2] (tetragonal Mo<sub>2</sub>FeB<sub>2</sub> type structure) at 100°C and 30 bar. The mass increase during hydrogenation corresponds to a hydrogen content of ~8 H atoms/formula unit (f.u.), i.e. the composition La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub>. Hydrogenation of the intermetallic leads to a monoclinic distortion and a lattice expansion of ΔV/V ~20%. The structure of the deuteride was solved using both synchrotron and neutron powder diffraction data. Preliminary X-ray measurements on a deuteride sample were performed at a Bruker D8 Advance diffractometer with CuKα radiation. The data showed a small monoclinic lattice distortion and were indexed in non-centrosymmetric space group P2<sub>1</sub>. To confirm the distortion, the same sample was studied by high-resolution synchrotron powder diffraction at the Swiss–Norwegian beam line (BM1) at ESRF (Grenoble, France). Based on results of the automatic indexing program DICVOL04 [3] a new monoclinic cell was found and assigned to centrosymmetric space group P2<sub>1</sub>/c. Structure refinement was carried out with the FULLPROF SUITE [4], starting with atomic coordinates as found by FOX [5]: 4 La, 4 Ni and 2 Mg sites, all on equipoint 4e of space group P2<sub>1</sub>/c. Absorption correction was applied by using the coefficient μ<sub>r</sub> = 0.807. In total, 57 parameters were refined: 1 scale factor, 6 background, 4 cell, 6 profile, 30 positional and 10 thermal parameters.

Neutron powder diffraction pattern were collected on a deuteride sample at SINQ (PSI, Villigen) using the high resolution powder diffractometer HRPT (deuterided sample, λ = 1.8857 Å). For structure solution, the metal atom positions were fixed at

the values determined by the previous synchrotron experiment and the deuterium atoms located by using FOX [5]. Within the 26 independent atomic positions in the cell, sixteen deuterium positions on equipoint  $4e$  in space group  $P2_1/c$  were located, corresponding to the composition  $\text{La}_2\text{MgNi}_2\text{D}_8$ . As their occupancy factors did not differ significantly from unity during preliminary structure refinements, they were fixed at this value during subsequent refinement cycles. The following 66 parameters were refined using the FULLPROF SUITE : 1 scale factors, 1 zero shift, 6 background, 48 positional and 4 thermal parameters, 4 profile and 2 microstrain parameters to model anisotropic line broadening.

The metal atom distribution is very similar to that of the tetragonal alloy, the atomic shifts being smaller than  $0.65 \text{ \AA}$ . There exist two sorts of deuterium atoms, one bonded to nickel, and the other not bonded to nickel. As shown in Fig. 1 those bonded to nickel (D11-D14, D21-D24, D31, D32, D41-43) constitute two types of polynuclear Ni-D complexes (**I**, **II**) in which all Ni atoms are surrounded in approximately tetrahedral configurations by both terminal (D11, D14, D31, D32, etc) and bridging (D12, D13, D23) deuterium ligands (called "complex" hydrogen/deuterium thereon).

**Figure 1** : Dinuclear  $[\text{Ni}_2\text{D}_7]$  (**I**) and tetranuclear  $[\text{Ni}_4\text{D}_{12}]$  (**II**) complexes in  $\text{La}_2\text{MgNi}_2\text{D}_8$  (bottom) and comparison with hydrogen-free  $\text{La}_2\text{MgNi}_2$  (top)

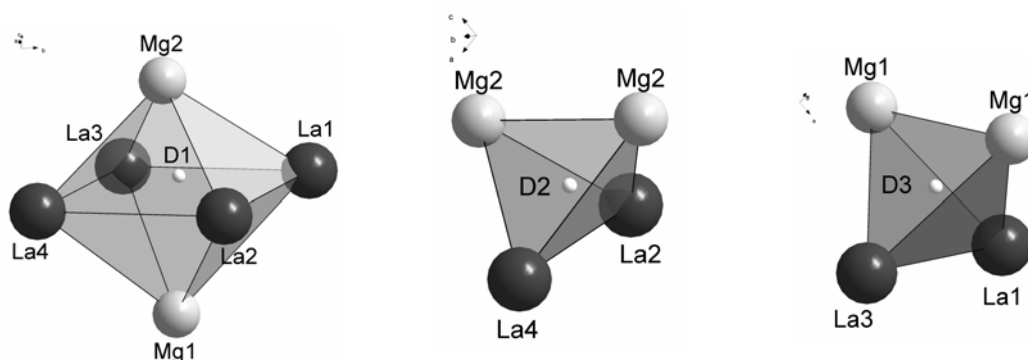


The smaller complex **I** consists of a pair of nickel centered tetrahedrons (Ni2, Ni4) joined over corners to dinuclear entities of composition  $\text{Ni}_2\text{D}_7$ , and the larger complex **II** of four nickel centered tetrahedrons (2Ni1, 2Ni3) joined over corners to tetranuclear entities of composition  $\text{Ni}_4\text{D}_{12}$ .

Given that the Ni-D distances within the complex anions (**I** : Ni-D=1.52-1.71 Å, **II** : Ni-D=1.50-1.70 Å) are much shorter than those between the anions (Ni3-D22=2.86 Å, Ni1-D42=2.88 Å), the complex anions are well isolated from each other. The bond angles deviate more-or-less from  $109^\circ$  (terminal: D-Ni-D  $\sim 92$ - $129^\circ$ , bridging: Ni1-D13-Ni3  $\sim 157^\circ$ , Ni1-D12-Ni3  $\sim 127^\circ$ ). In particular, the Ni-D-Ni bridge in **I** is significantly opened (Ni2-D23-Ni4  $\sim 125^\circ$ ) but far away from linear as reported for the Pt-H-Pt bridge in the dinuclear platinum complex anion  $[\text{Pt}_2\text{H}_9]^{5-}$  of  $\text{Li}_5\text{Pt}_2\text{H}_9$  [6].

The remaining D atoms (D1-D3, called "interstitial" hydrogen/deuterium thereon) are coordinated by lanthanum and magnesium only, As shown in Fig. 2 they have octahedral  $[\text{La}_4\text{Mg}_2]$ -type or tetrahedral  $[\text{La}_2\text{Mg}_2]$ -type configurations, and their

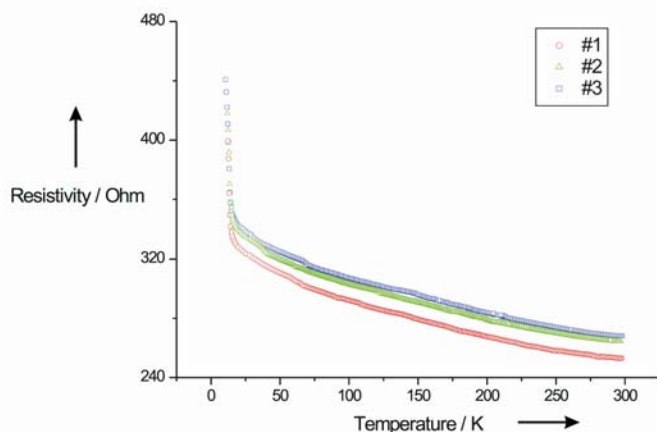
metal-deuterium distances are in the range Mg-D=1.92-2.77 Å and La-D= 2.27-3.22 Å, i.e. somewhat longer than those in LaMg<sub>2</sub>NiH<sub>7</sub> (Mg-D=1.82-2.65 Å, La-D=2.33-2.59 Å)



**Figure 2:** Metal coordinations of interstitial deuterium sites D1, D2, D3 in La<sub>2</sub>MgNi<sub>2</sub>D<sub>8</sub>

Altogether, the structural features and composition of La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> suggest a bonding description in terms of La<sup>3+</sup> and Mg<sup>2+</sup> cations and [Ni<sub>2</sub>H<sub>7</sub>]<sup>7-</sup>, [Ni<sub>4</sub>H<sub>12</sub>]<sup>12-</sup> and H<sup>-</sup> anions, corresponding to the limiting ionic formula 4.La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> = La<sub>8</sub><sup>3+</sup>Mg<sub>4</sub><sup>2+</sup>[Ni<sub>4</sub>H<sub>12</sub>]<sup>12-</sup> 2.[Ni<sub>2</sub>H<sub>7</sub>]<sup>7-</sup> 6H<sup>-</sup>. In other words, the electron requirement of the transition element in each complex (**I**: 34, **II**: 64 electrons) can be rationalized in terms of the 18 electron rule by attributing 2 center 2-electron bonds to terminal, and 3-center 2-electron bonds to bridging hydrogens. This model implies that Ni is essentially zero-valent, i.e. that the *d* bands are filled, and that the compound is diamagnetic and possibly insulating.

While the intermetallic compound La<sub>2</sub>MgNi<sub>2</sub> shows a very small electric resistance (~0.4 Ohm for a bulk sample of 40 mg) consistent with metallic behavior, the hydride La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> shows semiconductor behavior (see Fig. 3). However, in spite of the relatively well reproducible values a reliable value for the band gap could not be obtained because massive hydride samples were not available. The small discontinuities around 70 K do not originate from a lattice distortion as shown by a low-temperature neutron powder diffraction experiment on a deuteride sample.



**Figure 3:** Electric resistance versus temperature of a La<sub>2</sub>MgNi<sub>2</sub>H<sub>8</sub> powder sample as measured during three consecutive runs upon cooling.

In conclusion, we have reported the first case of a solid state metal hydride containing polynuclear hydride complexes based on a 3d-metal, i.e.  $\text{La}_2\text{MgNi}_2\text{H}_8$ . In contrast to the known nickel based metal hydrides containing exclusively mononuclear tetrahedral  $[\text{NiH}_4]^{4-}$  complexes with terminal H ligands such as  $\text{Mg}_2\text{NiH}_4$  and  $\text{MMgNiH}_4$  (M=Ca,Sr,Eu,Yb), it contains dinuclear  $[\text{Ni}_2\text{H}_7]^{7-}$  and tetranuclear  $[\text{Ni}_4\text{H}_{12}]^{12-}$  complexes displaying both terminal and bridging H ligands. The complexes are fully ordered. Their geometries are unique among complex metal hydrides and resemble remotely those of the  $[\text{Si}_2\text{O}_7]^{6-}$  and  $[\text{Si}_4\text{O}_{12}]^{8-}$  anions in soro- and ring silicates, respectively. The non-metallic character of the hydride is presumably due to the condensation of valence electrons into metal-hydrogen bonds of  $[\text{Ni}_2\text{H}_7]^{7-}$  and  $[\text{Ni}_4\text{H}_{12}]^{12-}$  complexes having closed-shell electron configurations (18-electrons). This is the fourth example of a hydrogenation induced metal-to-nonmetal transition in a T metal-hydrogen system. The challenge for future work is to synthesize more such systems, in particular those likely to display polynuclear or possibly heteronuclear complexes that are fully reversible. The prospects of finding such compounds are good, since the possible element combinations are numerous and not yet fully explored.

### References:

- [1] K.Yvon, G. Renaudin, C. M. Wei, and M. Y. Chou, *Phys. Rev. Lett.* **2005**, *94*(6) p. 066403-4.
- [2] R-D. Hoffmann, A.Fugmann., U.Ch. Rodewald, R. Pöttgen, *Z. Anorg. Allg. Chem.* **2000**, *626*, 1733-1738
- [3] A. Boultif , D.Louer, *J. Appl. Crystallogr.*, **2004**, *37*, 724-731.
- [4] J. Rodriguez-Carvajal, *FULLPROF version December 2005*, *ILL (unpublished)*. 2005.
- [5] V.Favre-Nicolin, R. Černý, *J. Appl. Cryst*, **2002**, *35*, 734-743.
- [6] W.Bronger, L. à Brassard., *Angew. Chem. Int. Ed. Engl*, **1995**, *34*, 898-900.

## Conference Report – EPDIC 10

### 10<sup>th</sup> European Powder Diffraction Conference

Uni Mail, Geneva, 1 – 4 September 2006

Workshops: 31 August – 1 September 2006

By Radovan Cerny (Radovan.Cerny@cryst.unige.ch)

The EPDIC conferences are a reference point for all researchers in the field of powder diffraction, and are regarded as an ideal setting for the presentation and discussion of new developments in powder diffraction instrumentation, analysis, and applications. It provides a forum for all powder diffractionists, whether their interests lie in theoretical developments or in the application of existing techniques, to meet and exchange ideas and expertise. EPDIC10 has continued in this tradition.

### Organization

The conference was organized jointly by the Swiss Society for Crystallography ([www.sgk-sscr.ch](http://www.sgk-sscr.ch)) and University of Geneva ([www.unige.ch](http://www.unige.ch)) in a building of the University called Uni Mail. The organizing committee was formed within the year 2004 and has met for the first time in November 2004. It worked till June 2006, when it passed the activity to the staff of EPDIC10, composed mainly from the co-workers of the University of Geneva, who have prepared and realized all the details of the on-site organization. The scientific secretariat of the conference was done by a professional organization SYMPORG ([www.symporg.ch](http://www.symporg.ch)).

### Scientific Programme

The scientific program of EPDIC10 was organized by the international Scientific Programme Committee (SPC), which is equal to the EPDIC committee ([www.mf.mpg.de/de/abteilungen/mittemeijer/epdic](http://www.mf.mpg.de/de/abteilungen/mittemeijer/epdic)) + invited guests. SPC has proposed 12 plenary lectures, of which 6 were kept and 20 microsymbiosia of which 15 were kept. The 16<sup>th</sup> microsymbiosium was created on the basis of submitted abstract. Each microsymbiosium had 5 speakers, which makes in total 80 oral presentations. The length of all microsymbiosia was identical (125 min), the typical distribution of the time was 25 min / speaker. The total number of poster presentations was 204. The program was finished by the beginning of June 2006.

### Plenary lectures:

**Simon Billinge** ( Michigan State University , USA):

The nanostructure problem, and some first steps to solve it.

**Irene Margiolaki** (ESRF, France):

Synchrotron X-ray powder diffraction as it begins to make an impact in structural biology.

**Vitalij Pecharsky** ( Ames Laboratory , USA):

In-situ powder diffraction involving high magnetic fields.

**Winfried Kockelmann** (ISIS, UK):

Advanced neutron powder diffraction techniques in archeometry.

**Andreas Leineweber** (MPI, Stuttgart, Germany):

Mechanisms and structural aspects of phase transformations in alloys of interstitial character - capabilities of powder diffraction.

**Olivier Thomas** (Université Paul Cezanne, Aix-Marseille III, France):

In-situ investigation by X-ray diffraction and wafer curvature of phase formation and stress evolution during metal thin film-silicon reactions.

## **Microsymposia:**

### TOTAL SCATTERING ANALYSIS

Chairpersons : **Thomas Proffen** (LANL Los Alamos), **Simon Billinge** (Uni Michigan)

### STRUCTURE DETERMINATION FROM A SINGLE POWDER DIFFRACTION PATTERN

Chairpersons : **Arnt Kern** (Bruker AXS), **Anton Meden** (Uni Ljubljana)

### POWDER DIFFRACTION AND BIO-MATERIALS

Chairpersons : **Bob von Dreele** (Argonne National Lab), **Marc Schiltz** (EPFL)

### COMBINING POWDER DIFFRACTION WITH OTHER METHODS

Chairpersons : **Lynne McCusker** (ETH Zurich), **Christian Baerlocher** (ETH Zurich)

### ENERGY STORAGE MATERIALS

Chairpersons : **Klaus Yvon** (Uni Geneva ), **Torbjorn Gustaffson** (Uni Uppsala)

### INSTRUMENTATION

Chairpersons : **Andrea Lausi** (ELETTRA), **Steve Hull** (ISIS)

### STRESS AND TEXTURE ANALYSIS

Chairpersons : **Udo Welzel** (Max Planck Institute Stuttgart ), **Matteo Leoni** (Uni Trento)

### STRUCTURE DETERMINATION FROM MULTIPLE POWDER DIFFRACTION PATTERNS

Chairpersons : **Bill David** (ISIS), **Jordi Rius** (CSIC Barcelona )

### VALIDATING STRUCTURES

Chairpersons : **Vitalij Pecharsky** (Ames Laboratory , USA), **Lachlan Cranswick** (Canadian Neutron Beam Centre)

### ANALYSIS IN CULTURAL HERITAGE AND FORENSIC SCIENCES

Chairpersons : **Eric Dooryhee** (CNRS), **Gilberto Artioli** (Uni Milano)

### DIFFRACTION ANALYSIS OF THE MICROSTRUCTURE OF MATERIALS

Chairpersons : **Paolo Scardi** (Uni Trento ), **Nathalie Audebrand** (Uni Rennes)

### NON AMBIENT CONDITIONS: PHASE TRANSITIONS/TRANSFORMATIONS

Chairpersons : **Andrew Fitch** (ESRF), **Robert Dinnebier** (Max Planck Institute Stuttgart)

### INDEXING

Chairpersons : **Lachlan Cranswick** (Canadian Neutron Beam Centre), **Christian Lengauer** (Uni Vienna)

### THIN FILMS, COATINGS AND SURFACES

Chairpersons : **Radomir Kuzel** (Uni Prague), **René Guinebretiere** (ENSCI Limoges)

## NEUTRON DIFFRACTION

Chairpersons : **Vladmir Pomjakushin** (Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institut, Villigen), **Juan Rodriguez-Carvajal** (ILL Grenoble)

## POWDER DIFFRACTION IN APPLIED RESEARCH

Chairpersons: **Daniel Louër** (Rennes), **Rob Delhez** (TU Delft)

### Workshops:

Four workshops were organized just before the conference from 31<sup>st</sup> August till 1<sup>st</sup> September:

- Pharmaceutical Applications of Powder Diffraction,
- Nano-materials and Powder Diffraction,
- Powder Diffraction Software Workshop: "Under the Bonnet",
- ICDD (International Centre for Diffraction Data) workshop.

An important part of EPDIC10 was the commercial exhibition, which took 133 m<sup>2</sup>. Majority from 12 exhibitors were the providers of powder diffraction equipment.

### Social Programme

Welcome party was organized first day of the conference in the main hall of Uni Mail. The highlight of the evening was the alphorn playing group **MYTHA** (*Hans Kenne*) with alpine sagas, myths and contemporary music woven into one unique musical experience. What the group achieved with alphorn, Büchel or Neverlure was beautifully unique. The vocal performance of invited singer-songwriter *Betty Legler* reached from elf-like reciting to powerful high-density jodelling and added yet another authentic dimension to MYTHA's alpine soundscapes.



The conference banquet was organized in the restaurant situated on the top of the World Meteorological Organization with a beautiful view on the Geneva lake and the Alps. The evening was animated by the music group **Atrio+** playing the swing from the 40's, the be-bop, latin-jazz and more actual tendencies.

### Participants and Supporting

The final number of participants presented at EPDIC10 was 374. The most represented country was Switzerland with 55 participants followed by Germany (54), France (37), UK (26), Russia (22), Italy (21), USA (21) etc. **52 students** and **early researchers** were supported by the conference (support to travel and

accommodation expenses, early student registration fee). The total amount of the support was approx. **30 kCH** thanks to various organizations. Besides the exhibitors and student supporters the conference was well recognized by general sponsors and donators who all contributed to the success of EPDIC10. The full list of the supporting organization can be found on [www.sgk-sscr.ch/EPDIC10](http://www.sgk-sscr.ch/EPDIC10).

### **EPDIC Award: Irene Margiolaki**



The **EPDIC award** is assigned at each EPDIC Conference and honours outstanding scientific achievement by young scientists in the field of powder diffraction. The award winner is invited to present a plenary talk at the next European Powder Diffraction Conference. The EPDIC10 award was given to **Irene Margiolaki** (ESRF, Grenoble, France) for her important contribution to the application of powder diffraction in the research on bio-molecules.

### **Conference Summary**

EPDIC10 conference and its workshops were a great success, thanks to the perfect infrastructure of the conference site (Uni Mail), responsible work of all people involved (organizing committee, staff, personnel of Uni Mail, scientific programme committee) and generous support of sponsors, donators and supporting organizations. I thank to all of them, especially to the staff members (the list of the staff members can be found on [www.sgk-sscr.ch/EPDIC10](http://www.sgk-sscr.ch/EPDIC10)) for their enthusiastic work without regarding the time and date (the conference was organized during the weekend).

The proceedings of EPDIC10 will be published as a special issue of Zeitschrift fuer Kristallographie ([www.zkristallogr.de](http://www.zkristallogr.de)) within the year 2007.

## General Assembly 2006, Berne

### Minutes of the General Assembly

1. Approval of the Agenda (Steurer)

*The agenda has been accepted without changes.*

2. Minutes of the General Assembly on Oct 13 2005, Lausanne

The minutes were published in the SSCr Newsletter 67. *They have been approved without changes.*

3. Reports from the SSCr:

3.a. Annual Report of the President 2006 (Steurer)

### General Information

- Our member and former president Erwin Parthé died on August 28th, 2006, in Geneva, at the age of 78. Obituaries will be published in Zeitschrift für Kristallographie (Grin/Paufler) and Acta Crystallographica (Jeitschko?).
- Our member and former president Edgar Ascher died in Geneva on July 28, 2006, at the age of 85. An obituary (Grimmer) was published in Newsletter 69.
- Our former member Hans Günthard died on February 2nd, 2006 at the age of 90. A short notice was published in our Newsletter No 67.
- On February 27th, 2006, we commemorated the 100<sup>th</sup> birthday of Fritz Laves, who was professor at ETH and University of Zurich from 1956 to 1976. An article (written by D. Schwarzenbach) appeared in our Newsletter No. 68, Zeitschrift für Kristallographie published a special issue on that occasion (Guest Editor Yuri Grin).
- Our member Tim Richmond received the Marcel Benoist Prize (CHF 100'000) for his structural studies of nucleosomes.
- Our member Artem Oganov will receive the Latsis Prize of the ETH (CHF 25'000) for his work in computational crystallography.
- Our member Hans Grimmer retired end of SS 2006.
- Our member Hans-Beat Bürgi will retire end of WS 2006/07.

## **Work of the committee**

The committee (President W. Steurer, Vice-President H.J. Scheel, Secretary and ECA representative J. Schefer, Treasurer M. Hennig, Marc Schiltz, Klaus Yvon) met twice in 2006, on 27.1.06 and on 9.6.06 in Berne, in between the committee members communicated per email. The main points dealt with were

- financial support for four young scientists (see item 8.);
- decision on new rules for travel grants for young SSCr members (see item 8.);
- discussion of possible actions concerning the future of crystallography in Switzerland.  
The main result was that we should strengthen the links to biological crystallography and that we should increase our visibility. Appropriate measures could be to create a new section 'Biological Crystallography' within the SSCr and to organize our annual meetings together with other organisations in Switzerland and in neighbouring countries, respectively (DGK, SLS,...).
- discussion of the future of the Section Crystal Growth (SKT). Presently, 24 members of the SGK/SSCr have registered as members of this section. It is headed by Hans J. Scheel. The finances are managed by Katharina Fromm. One of the major activities is the organization of the international Beatenberg workshops (IWCGT-3/2006 and IWCGT-4/2008). Katharina Fromm has been nominated as new chairperson of the SKT.
- Comments: Reorganisation of the section SKT, e.g. by introducing special interest groups (SIGs) without a special organization form would be more appropriate; ask in addition biological crystallographers whether they would like to have their own SIG.  
The general assembly asks for a proposition for the next meeting in 2007.
- Three editions of our newsletters were published:  
67 (3/2006), 68 (7/2006) and 69 (9/2006). They are available also on internet.

## **Contacts to SANW/ASSN**

Radovan Cerny (as past president) represents the SSCr in the Senate (2006-2008) and Walter Steurer in Section I of the SANW/ASSN, which contributed this year as before CHF 1000 for travel grants for young scientists, CHF 2500 for the organization of the annual meeting and CHF 500 for ECA delegates.

International Conferences in Switzerland

EPDIC-10 took place in Geneva, Sept 1-4, 2006. Radovan Cerny was Chairman of the Organizing Committee for this very successful conference.

3.b. Report of the treasurer (Hennig)  
accepted without comments (financial report: page 22 in this newsletter)

3.c. Report of the auditors (Bärlocher/Schenk)  
*accepted without comments.*

4. Budget 2007 and membership fees 2007 (Hennig)  
The membership fee stays unchanged (30 CHF regular, 10 CHF students)  
accepted without comments (details see on page 24 in this newsletter)

Status of payments of membership fees due:

September 2006: 69% paid (117 von 171 Mitgliedern)

September 2005: 71% paid (119 von 167 Mitgliedern)

5. Reports from the Section Crystal Growth (Scheel is abroad, no report available)

5.a. Treasurer (K. Fromm is excused due to the start of the semester, financial report on page 25 of this newsletter)

5.b. Auditors

6. Budget 2007 of the Section Crystal Growth (see page 25, not presented at the meeting, K. Fromm excused)

7. Report of the delegate to the ECA Council Meeting Leuven (Schefer)

The ECA meeting in Leuven elected a new board (see minutes of the ECA board on page 29 in this newsletter). The next ECA conferences will take place in Marrakech (2007) and Istanbul (2009). Individual ECA members profit of reduced registrations fees.

8. Award of travel grants (Steurer)

Grants given in 2006 (CHF 2500 in total):

Ivan Orlov EPFL Lausanne	ECM 23, Leuven, Belgium	11-14.8.2006 (invited talk)	750.--
Philippe Kocian EPFL Lausanne	ECM 23, Leuven, Belgium	11-14.8.2006 (Poster)	500.--
Aude Escande University Geneva	6 <sup>th</sup> Int. Conf. on f Elements, Wroclaw, Poland	4-9.9.2006	500.--
Jean-Noël Chotard, University Geneva	MH 2006, Hawaii, USA (Metal Hydrides)	1.-6.10.2006	750.--

The board agreed on **new decision rules for travel grants** for young SGK/SSCr members:

- Only members of the SGK/SSCr can be financially supported.
- **Student members** can get up to CHF 500 for a poster presentation and CHF 750 for an oral presentation.
- **Postdocs** can be supported only for oral presentations with a maximum of CHF 500.
- Per institute and year, only **two persons** can be supported.

- A 1-2 page scientific contribution to the SGK/SSCr newsletter is expected.

#### 9. Election of the section head of Section Crystal Growth SKT/SCT (Steurer)

The committee unanimously proposes Katharina Fromm, former assistant professor (tenure track) at the Department of Chemistry, University Basle, now professor at the University of Fribourg.

*accepted without comments*

#### 10. Election of the Auditors (Steurer)

We highly appreciate the keenness of the present auditors, Ch. Bärlocher (ETH Zurich)/K. Schenk (EPFL), and nominate them again.

#### 11. Amendments to the by-laws of the SSCr (Steurer)

11.a. Discussion on the creation of New Sections (working groups, i.e. Arbeitskreise) such as Section Biological Crystallography (SBC).

11.b. Further minor modifications to be worked out by the committee.

#### 12. Annual Meeting 2007 (Steurer)

The meeting will be held together with the SLS user meeting on Sept 10-12, at PSI.

*accepted without objections*

#### 13. Varia *not used*

#### 14. Closing

W. Steurer closes the general assembly and thanks again for joining the meeting.

**Financial Report SGK/SSCr**  
M .Hennig

**SGK/SSCr Budget 2006**

(in CHF)

**Status 1.1.2006** **13'450.00**

**Credits 2006:**

	<b>Budget</b>	<b>(Actual)</b>
Membership dues (152-F, 7-J, 11-S)	5'610.00	(4'610.01)
ECA individual dues (7 members)	105.00	(75.00)
Interest (est.)	120.00	(0.00)
Bank charges	0.00	(9.60)
SANW for Annual Meeting 2006	2'500.00	(0.00)
SANW for 10th Eur. Powder Diffr. Conf. EPDIC 10	4'500.00	(0.00)
SANW for ECA delegate 2006	500.00	(0.00)
SANW Young Scientists travel grants	1'000.00	(1'000.00)
Loterie Romande (for EPDIC 10)	0.00	(7'000.00)
<b>Total Income 2006</b>	<b>14'335.00</b>	<b>(12'694.61)</b>
<b>Cash on Hand – 2006 (as of 9.10.06)</b>		<b>353.80</b>

<b>Debits 2006:</b>	<b>Budgeted</b>	<b>Actual</b>	
Sekt. Kristallwachstum (2006)	600.00	(600.00)	
Membership dues to SANW(171 members)	1'169.00	(1'197.00)	
Annual meeting 2006	2'500.00	(0.00)	
Loterie Romand (EPDIC 10)	0.00	(7'000.00)	
Travel Grants to Young Scientists	1'750.00	(1'250.00)	
Travel Grants for ECA delegate (2006)	1'000.00	(0.00)	
ECA dues (national + 7 members) + bank	217.00	(0.00)	
10th Eur. Powder Diffr. Conf. EPDIC 10	4'500.00	(0.00)	
Travel Expenses Exec. Comm. and Auditors	600.00	(0.00)	*)
SWITCH (Web address „sgk-sscr.ch“)	35.00	(0.00)	*)
Cash withdrawal	0.00	(400.00)	
Bank Charges	125.00	(18.90)	
Postage Charges	55.00	(0.00)	
Withholding Tax (35%)	42.00	(0.00)	
 Paid out of Cash on Hand			*)
 Total Expenses	12'593.00	(10'465.90)	
Income – Expenses	1'742.00	(2'228.71)	
Starting Balance + Income – Expenses	15'192.00	(15'678.71)	
Est. UBS Balance <b>31.12.2006</b>	15'192.00	(15'678.71)	

### **Cash on Hand – 2006**

**Status 1.1.2006** **353.80**

#### **Credits 2006:**

Membership dues (3 persons, 4 annual fees) 120.00  
Drawing from UBS account 400.00

**Total Income** **520.00**

#### **Debits 2006:**

SWITCH (Web address „sgk-sscr.ch“) 35.00  
Travel Expenses, Executive Committee 158.00

**Total Expenses** **193.00**

**Income – Expenses** **+327.00**

**Cash on Hand 9.10.2006** **(353.80+327.00)** **680.80**

### **Total SGK/SSCr Assets 2006**

	<b>31.12.06</b>	<b>9.10.06</b>
UBS account	15'192.00	15'678.71
CS account	17'147.00	16'998.40
Cash on hand	200.00	680.80
<b>Total</b>	<b>32'539.00</b>	<b>33'357.91</b>

## SGK/SSCr Budget 2007

### Budget Credits 2007:

Membership dues (152-F, 7-J, 11-S)	5'580.00
ECA individual dues (7 members)	105.00
SANW reimbursement for Annual Meeting 2007	2'500.00
SANW reimbursement for ECA delegate 2007	1'000.00
SANW young scientists travel grants	1'000.00
Interest (est.)	120.00

**Total Income SGK/SSCr 2007** **10'305.00**

### Budget Debits 2007

Sekt. Kristallwachstum (2007)	600.00
Membership dues to SANW (170 members)	1'190.00
Annual meeting	2'000.00
Travel Grants to Young Scientists	1'500.00
Travel Grant for ECA delegate (2007)	1'000.00
ECA dues (national + 7 members + bank charges)	217.00
Travel Expenses Exec. Committee and Auditors	600.00 *)
SWITCH (Web address „sgk-sscr.ch“)	35.00 *)
Postage charges	55.00
Bank charges	125.00
Withholding Tax (35%)	42.00

**Total SGK/SSCr Expenses 2007** **7'364.00**

Income – Expenses (profit) 2'941.00

Starting Balance Total SGK Assets 1.1.2007 **32'539.00**

+ Income – Expenses 31.12.2007 **35'480.00**

paid out of cash-hand \*)

## Financial Report Section Crystal Growth (SKT)

K. Fromm

### SKT Finanzen 2006:

31.12.2005		5'176.95
12.07.2006	SGK/SSCr	600.00
today (21.11.2006)		<b>5'776.95</b>

### SKT Budget 2007:

#### Credits 2007:

SGK/SSCr		600.00
Total Income 2007		<b>600.00</b>

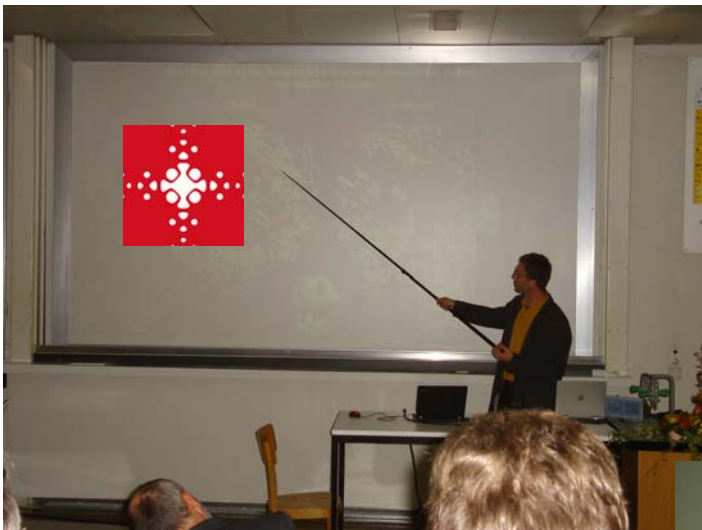
Geplante Ausgaben:

eventuell im Rahmen der Organisation des nächsten Beatenberg Workshops, aber noch offen.

**Impressions from the Annual Meeting of the SGK/SSCr and the social dinner (Berne, 2006)**







**SGK/SSCr**  
**Berne 2006**

Photos: courtesy of Denis Prodius



# Minutes of the ECA Meeting in Leuven, Belgium

(from ECANEWS, giuseppe.filippini@istm.cnr.it)

## First session: 7 August, 2006

### 1. Opening

#### 1.1 Welcome to Council and Guests

The Chairman welcomed the Councillors, the observers and the guests.

#### 1.2 Application for membership

The Secretary informed that no applications have been received. The President introduced the observer from Armenia and invited her to say a few words. Dr Bezirganyan reported briefly on the situation of crystallography in her Country and thanked the EC and the Council for the opportunity of attending the meeting. Contacts with potential members of the ECA have been planned, with the presence of members of the EC at the national meetings.

#### 1.3 News and information from the Executive Committee.

##### 1.3.1 Max Perutz Prize

The Prize has been given, during the Opening Ceremony, to Eleanor Dodson, "for developing, implementing, teaching and applying the best tools available to produce macromolecular structures of highest quality".

##### 1.3.2 Felix Bertaut Prize

The foundation of the Prize in cooperation with the European Neutron Scattering Association (ENSA) was announced for young scientists under 35. Crystallographers and neutron diffraction researchers will receive the prize in a sequence to be defined. The first award will be distributed during the ENSA meeting at Lund in July 2007.

##### 1.3.3 ECANEWS

The President thanked the webmaster, Professor Massimo Nespolo, for his dedicated contribution in improving the site. Professor Nespolo stressed that every Country should have a responsible liaison in order to speed up the flow of information. As a start the Councillors themselves will act in this office. Links with the National and SIGs' websites will be further implemented.

### 2. Former e-mail decisions

No decisions were taken by e-mail between the Council in Firenze and the present one in Leuven.

### 3. Annual Reports by the Executive Committee (Aug. 2005 - 31 Dec. 2005) and preliminary progress reports (up to Aug. 2006)

#### 3.1 Report by the President

Professor Fuess referred to his report sent to all Councillors(enclosed).

#### 3.2 Report by the Vice-President on sponsorship of meeting and schools.

During the term 2003-2006, the main activities of the Vice President were focused (i) on coordination of the ECA program to support crystallographic schools and conferences, and (ii) on attempts to establish contacts with new national members.

Ad (i): A set of rules have been worked out for supporting the participation of young scientists in crystallographic schools and conferences. Those rules were discussed during ECA Council Meetings and are enclosed as a document entitled "Operational guidelines for supporting European workshops, schools, and conferences on crystallography by ECA". These Guidelines have been used to evaluate applications for support, to disburse the funds, and to collect reports. Overall, 14 meetings were supported for the total amount of 18000 Euros (2004: 3 meetings, 4000 Euros; 2005: 5 meetings, 7000 Euros; 2006: 6 meetings, 7000 Euros). At the time of the ECA Council Meeting in Leuven, reports from organizers of all closed meetings have been obtained. They are available from the Vice President on request. A summary of all grants awarded during the term 2003-2006 is enclosed.

Ad (ii): Letters have been sent to the crystallographic communities in Romania, Belarus, and Lithuania. As a result, an observer from Belarus attended the ECA Council Meeting in Budapest, August 2004.

### 3.3 Report by the Secretary

Dr Filippini thanked the Councillors for many fruitful contacts during the six years of office and pointed out some aspects which may be overcome only with their help. The more the Association is growing, the more the Secretary needs the help of everybody to keep the pace with the dissemination of the information. And this is particularly needed when a new Secretary takes office.

### 3.4 Report by the Treasurer

Professor Duarte reported on the budget. Sending on time annual invoices to the Councillors improved the payments.

The situation of the budget is fine, and will even improve if the ECM's organizers will continue to give some money to the ECA, as it has been done so far by the organizers of Nancy and Budapest ECM's.

Dr Kuzel reported on the IM's fees collection which resulted in more than 200 regular members. The five-year fee (€ 50), decided in order to simplify the procedures and save money, seems to work both by credit card payments and money transfer.

## 4. Approval by the Council of the submitted accounts (re 3.3)

One of the auditors, Professor Garcia-Granda, read the report with approval.

*The Councillors approved the audited accounts for 2005.*

### 4.1 Auditors for 2006

No decision has been taken. Proposals will be put forward by the new EC and approved by the Councillors according to the TVP.

### *Pre 7. Elections for President and other Officers*

At the Chairman's request, the Council agreed to listen to the statements of all the candidates for the new Executive Committee.

Professors Helliwell, Larsen, Kuzel, Effenberger, Garcia-Granda, Roodt, van Meervelt, Wilson and Doctors Bombicz and Mealli said a few words on their aims and wishes should they be elected.

## 5. Reports regarding SIG's

The reports of the Scientific Interest Groups were accepted as far as available.

## Second session: 9 August, 2006

### 6. Reports regarding ECM's

#### 6.0 Relationship between ECA and the ECM's

It seems to the Council that the relationships between the ECA and the ECM work properly: the presence of two members of the Executive Committee ensure both the scientific level and the continuity.

#### 6.1 ECM-23 (2006) Leuven ([www.ecm23.be/](http://www.ecm23.be/))

Professor Van Meervelt gave more details on ECM-23 (2006).

From 4 to 6 a Satellite on "Mathematical Crystallography" has been held:

[<http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm>] with 50 participants.

The format follows that of previous ECMs, opening and welcome on 6<sup>th</sup>. From 7 to 10: in the morning 2 parallel Keynote Lectures + 6 parallel Microsymposia, the same (but reversed) in the afternoon + poster session.

The conference dinner on 10<sup>th</sup> and the excursion on 11<sup>th</sup> are included in the registration fee.

Attendance is of more than 800 participants.

#### 6.2 ECM-24 (2007) Marrakech

Professor Thalal and a representative of the organizing secretariat in Marrakech gave details on the site and fees of ECM-24 in Marrakech. The meeting will take place from 22 to 27 August, 2007 at the Palais des Congrès ([www.mansoureddahbi.com](http://www.mansoureddahbi.com)), with opening ceremony and welcome cocktail on the 22<sup>nd</sup> evening, four full days (23-26) for Keynote Lectures, Microsymposia, Poster Sessions and exhibitors, and the excursion on 27<sup>th</sup>. Conference dinner (26<sup>th</sup>) and excursion are included in the registration (ordinary before March 31<sup>st</sup> 2007/late 370/440€, ECA IMs 350/420 €, student packet = registration + BB for 7 nights 350/400 €, accompanying 120€). Grants are planned to be offered not only for students, but also for researchers from developing countries.

The website, which is continuously updated, is at [www.ecm24.org/](http://www.ecm24.org/).

### 7. Elections for President and other Officers

#### 7.1 Election for President

No other proposals being received, Professor **John R. Helliwell** has been declared the new President.

#### 7.2 Election for Vice-President

No other proposals being received, Professor **Sine Larsen** has been declared the new Vice-President.

#### 7.3 Election for Secretary

No other proposals being received, Dr **Petra Bombicz** has been declared the new Secretary.

#### 7.4 Election for Treasurer

No other proposals being received, Professor **Radomir Kuzel** has been declared the new Treasurer.

#### 7.5 Elections for Ordinary Members of the Executive Committee

The six candidates (Effenberger, Garcia-Granda, Mealli, Roodt, van Meervelt, Wilson) were put under secret ballot. Professor Duarte and Jaskolski acted as tellers. After two votes, the elected were: **Santiago Garcia-Granda, Andreas Roodt** and **Luc van Meervelt**.

8. The ECA : what to do - where to go

Discussion regarding rules and future proceedings

Operational guidelines for supporting European workshops, schools and conferences on crystallography by ECA (available from ECA by request)

9. Any other business

The Chairman thanked all the participants for the useful discussion.

..A vote of thanks was given by the Councillor for Russia for all the EC Members who finished their term.

10. Close

Giuseppe Filippini, Secretary

Hartmut Fuess, President

## News for and from Members

### **We welcome the following new members of the SGK/SSCr:**

Ms. Annasara Dahlström  
(EPF Lausanne, LCR2, SB IMPC, 1015 Lausanne, Thesis Student)

Dr. Olga Smirnova (Laboratoire de Crystallographie, 24 Quai Ernest-Ansermet,  
Université de Genève, 1211 Genève)

Mr. Alexandre Manton (Department of Chemistry, University of Basel,  
Klingelbergstrasse 80, 4056 Basel, Thesis Student)

Mr. A.K. Sachan (JNU Uttar-Pradesh, India, Master Student)

### **In Memoriam J.J. Burckhardt**

Prof J.J. Burckhardt (Titularprofessor der Universität Zürich) ist am 5. November in seinem 104. Altersjahr gestorben. Er hat unter anderem auch durch seine im Birkhäuser Verlag erschienenen Bücher

- Die Bewegungsgruppen der Kristallographie (1947) und
  - Die Symmetrie der Kristalle (1988)
- einen wichtigen Beitrag für die Kristallographie geleistet.

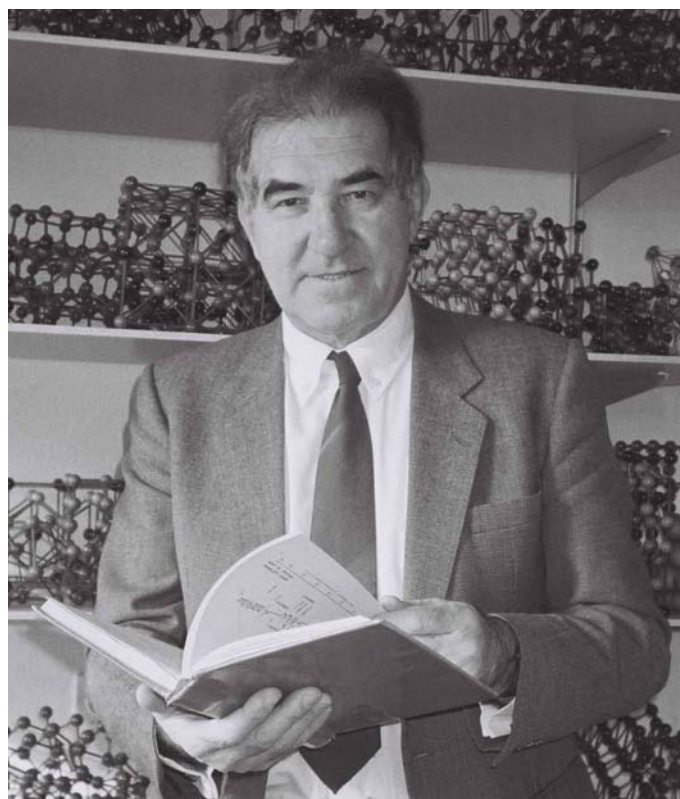
„Nach der Matura studierte J.J. Burckhardt von 1922 – 1927 Mathematik an den Universitäten Basel, München, Hamburg und Zürich, wo er im Jahre 1927 promovierte. Er blieb an der Universität Zürich; ab 1933 war er Privatdozent, 1945-1970 Oberassistent. J. J. Burckhardt kam über die reine Mathematik zur Kristallographie. Mitbestimmend war sicher seine grosse Liebe zur Natur – er war ein begeisterter Wanderer und Bergsteiger. J.J. Burckhardt war Ehrenmitglied der Naturforschenden Gesellschaft in Zürich und der Schweizerischen Mathematischen Gesellschaft....“

(Auszug aus Klappentext „Die Symmetrie der Kristalle“ (1988), J.J. Burckhardt, ISBN 3-7643-1918-6, Abdruck mit Erlaubnis des Birkhäuser Verlages Basel, Boston, Berlin)

## In Memoriam Erwin Parthé (1928-2006)

By Karin Cenzual (photo by R. Gladyshevskii)  
(Karin.Cenzual@unige.ch)

Erwin Parthé was born in Vienna, and obtained a Ph.D. degree in physical chemistry from the University of Vienna in 1954 under the guidance of Professor H. Nowotny. During the years 1955-1960 he enlarged his scientific experience as a postdoctoral fellow, then lecturer at the Massachusetts Institute of Technology. He continued his career as professor of materials science at the University of Pennsylvania from 1960 to 1970, with a stay as a guest professor of physics at the University of Grenoble 1966-1967. In 1970 he was appointed professor of structural crystallography at the University of Geneva. After his retirement in 1993 he went on publishing scientific papers and giving various courses on crystal chemistry around the world.



In addition to ca 250 scientific papers on crystal chemistry and crystal structures of inorganic and intermetallic compounds, Erwin Parthé has written three books on inorganic crystal chemistry, translated into various languages. He was president of the Swiss Society of Crystallography from 1978 to 1981. Amongst other distinctions he was awarded a *Doctor honoris causa* from the University of Savoy in 1980, and in 1991 he received the *William Hume-Rothery Award* of the American Minerals, Metals and Materials Society. The mineral parthéite,  $\text{Ca}_2\text{Al}_4\text{Si}_4\text{O}_{15}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$ , is named after him. In 1990 he was made honorary professor at the University of Vienna, and in 1993 at the University of Geneva.

Before switching over to intermetallic compounds, Erwin Parthé focused on tetrahedral structures, and remained until the end deeply interested in the relation between the information concerning the electronic configuration contained in the chemical formula and the crystal structure. He developed a system to standardize the crystallographic data of inorganic structures in order to better compare them (STRUCTURE TIDY), and created a database of structure types adopted by inorganic compounds (TYPIX). He is also the coauthor of one of the classical tools for powder diffraction, the program LAZY PULVERIX.

Through the years, he trained several PhD students and invited researchers. It was a hard school where so-called 'sloppism' was banned, concerning everything from

rigorous scientific work to missing commas. However, he never neglected the human side, and, because most of us were foreigners and had our families far away, he became like a second father to some of us. I remember in particular his more or less successful attempts to teach downhill skiing (a must in both Switzerland and Austria) to assistants, some of whom had never seen snow before, but also Christmas dinner at his home.

Besides his passion for crystallography and crystal chemistry, Erwin Parthé had several other activities and got easily interested in any kind of topic from Arab language to heating installations. Predominant hobbies were mountain hiking, skiing and music, in particular opera, well connected with his Austrian origin. He effectively remained 'ein Wiener', but also enjoyed traveling and a displacement was always worth a, sometimes relatively long, detour to visit some interesting site. He came back enthusiastic from countries such as Cuba, Mexico, Bolivia, China, Iran, etc., impressed both by the beauty of the country and the students' interest in crystal chemistry. The trips were, however, not always free of problems and the Laboratory once got a telephone call from an embassy in a South American country asking if we knew a certain Parthé, who had lost passport and money, but pretended he was professor at Geneva University.

Erwin Parthé deceased on August 28, 2006, in Geneva, at the age of 78 years, after a long and brave fight against cancer. Our condolences go to his wife Katrin and his daughters Claudia and Sylvia.

### **Missing Addresses of SGK/SSCr Members**

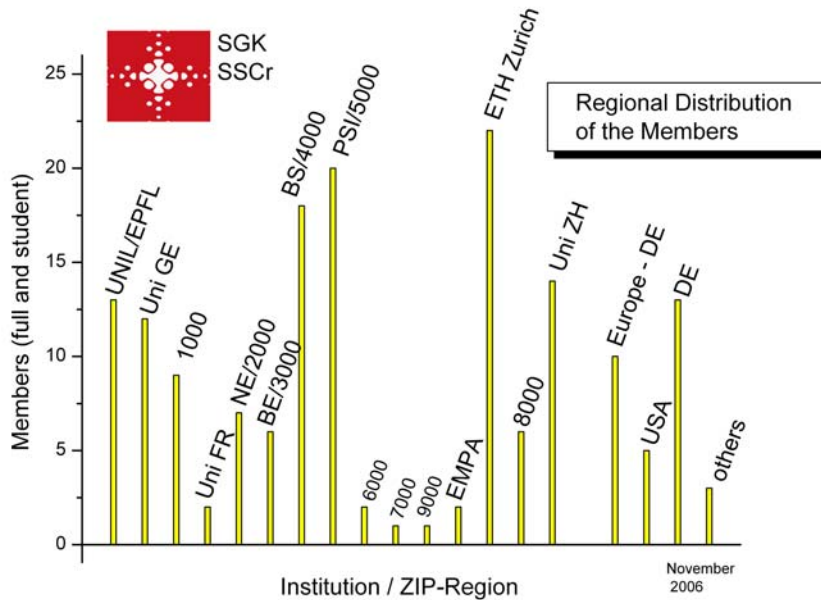
We have problems to contact the following members (last known affiliation in brackets):

- Jean Philippe Rapin (Laboratoire de Crystallographie, Université de Genève)

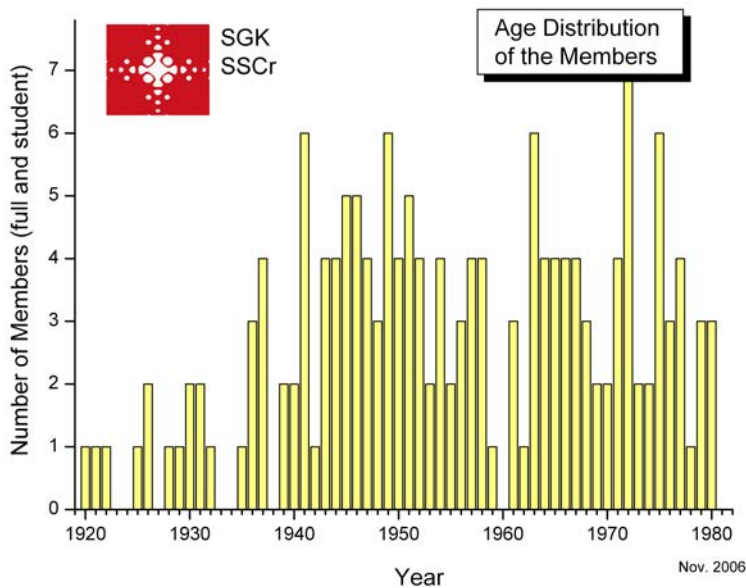
If the new address is known to you, please send an E-mail or FAX to the editor.

## Statistics on SGK/SSCr

On November 15, our society was counting 167 active members (regular and students, without honorary members). The statistics below shows the regional distribution (as a function of ZIP codes, some universities and research laboratories are listed as separate units. Every member is counted only in one group).



The age distribution of our society stays relatively constant (with one significant gap). It is very positive that we gained a number of new young scientist in the past few years.



# The 2007 Walter Halg Prize of the European Neutron Scattering Association



## The Walter Halg Prize

The prize was made available to the European Neutron Scattering Association (ENSA) by a donation from Professor Walter Halg who is the founder of neutron scattering in Switzerland. The Prize is awarded biennially to a European scientist for outstanding, coherent work in neutron scattering with long-term impact on scientific and/or technical neutron scattering applications. The previous Prize winners were F. Mezei (1999), J. Brown (2001), R. Cowley (2003), A. Furrer and H.U. Gudel (2005). The fifth award of the Prize (10'000 CHF) is to be made at a special ceremony and session at the 4<sup>th</sup> European Conference on Neutron Scattering (ECNS 2007), 25-29 June 2007, Lund, Sweden. Information on previous laureates are available on the ENSA web-site (<http://neutron.neutron-eu.net/n-ensa>).

## Selection Committee

Nominations for the prize will be considered by a Selection Committee which consists of authorities representing the major scientific disciplines. It includes acknowledged experts both in neutron scattering and from outside the neutron scattering community. Membership in the Selection Committee is obtained by invitation extended by the ENSA Committee.

## Call for Nominations

Nominations for the 2007 Walter Halg Prize of the European Neutron Scattering Association (ENSA) may be submitted by European scientists as individuals or on behalf of a Division, Section or Group. To establish a high standard it is necessary that the Committee receive proposals which represent the breadth and strength of European neutron scattering.



Nominations should include the motivation for the award, a brief curriculum vitae of the nominee and a short list of major publications. Letters of support from authorities in the field which outline the importance of the work would also be helpful. Nominations for the Prize will be treated in confidence and although they will be acknowledged there will be no further communication. Previous nominations have to be up-dated and resubmitted.

## Deadline

Nominations should be sent before **2 March 2007** to the Chairman of the Selection Committee, preferably by electronic mail in pdf format:

Dr. Peter Allenspach  
*ENSA Chairman*  
Paul Scherrer Institute  
CH-5232 Villigen PSI, Switzerland  
Phone: +41 56 310 2527  
Fax: +41 56 310 2939  
E-mail: [peter.allenspach@psi.ch](mailto:peter.allenspach@psi.ch)

## Call for Proposals

**Beside normal proposals, most facilities allow urgent beam time requests.  
Please check directly with the facility.**

<b>Facility</b>	<b>Deadline(s)</b>	<b>Link</b>
<b>SLS: Swiss Light Source</b> All except PX lines Protein beam lines (PX)	March 15, Nov. 15 Feb. 15, June 15, Oct. 15	user.web.psi.ch user.web.psi.ch
<b>SINQ: Swiss Spallation Neutron Source</b> All instruments except irradiation	May 15, Nov. 15	user.web.psi.ch
<b>SμS: Swiss Muon Source</b> All instruments	Dec. 5	user.web.psi.ch
<b>ESRF: European Synchrotron</b> All instruments, long term proposals All instruments, short term proposals	Jan. 15 March 1, Sept. 1	www.esrf.fr www.esrf.fr
<b>SNBL: Swiss Norwegian Beam Line</b>	March 1, Sept. 1	www.esrf.fr/ exp_facilities/BM1A
<b>ILL: Institut Laue Langevin</b> All instruments	mid September, February	www.ill.fr
<b>FRM-II</b> All instruments	26. Jan, 17. Aug.	user.frm2.tum.de

## Calendar of Forthcoming Meetings

			<b>Abstract Deadline</b>
<b>2007</b>			
Jan 14-19 New date: July 15-20, 2007	Havana Cuba	International School on Mathematical and Theoretical Crystallography <a href="http://www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm">www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm</a>	
Feb. 19-22	Barcelona Spain	PPXRD-6 The Pharmaceutical Powder X-ray Diffraction Symposium, <a href="http://www.iddd.com/ppxrd">http://www.iddd.com/ppxrd</a>	Expired
Feb. 20-21	Zürich CH	Annual Meeting of the Swiss Physical Society <a href="http://www.sps.ch">http://www.sps.ch</a>	Expired
March 5-9	Bremen Germany	Deutsche Gesellschaft für Kristallographie Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, Jahrestagung <a href="http://www.dgk-dgkk-2007.uni-bremen.de/">http://www.dgk-dgkk-2007.uni-bremen.de/</a>	<b>15.12.06 (extended)</b>
April 18-21	Engelberg CH	Landscape Development in Mountain Regions <a href="http://www.scnat.ch/d/Aktuell/Veranstaltungen/">http://www.scnat.ch/d/Aktuell/Veranstaltungen/</a>	
April 26-29	Dongguang China	ICANS XVIII – Neutron Spallation Sources <a href="http://icans-XVIII.ac.cn">http://icans-XVIII.ac.cn</a>	Dec. 31, 2006
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties <a href="http://www.crystalerice.org/2007.htm">http://www.crystalerice.org/2007.htm</a>	Expired
June 25-29	Lund Sweden	4 <sup>th</sup> European Conference on Neutron Scattering <a href="http://www.ecns2007.org">http://www.ecns2007.org</a>	Feb. 15, 2007
June 15-29	Istanbul Turkey	Nanoscaled Magnetism, ICNM-2007 <a href="http://web.gyte.edu.tr/ICNM/2007">http://web.gyte.edu.tr/ICNM/2007</a>	Feb. 1, 2007
July 21-26	Salt Lake City, USA	Annual Meeting of the American Crystallographic Society <a href="http://aca.hwi.buffalo.edu">aca.hwi.buffalo.edu</a>	March 1, 2007
August 5-11	Turin Italy	41 <sup>st</sup> IUPAC World Chemistry Congress <a href="http://www.IUPAC2007.org">http://www.IUPAC2007.org</a>	to be announced
August 13-17	Manchester UK	9 <sup>th</sup> Int'l Conference on Biology and Synchrotron Radiation <a href="http://www.srs.ac.uk/bsr2007">www.srs.ac.uk/bsr2007</a>	March 31, 2007
August 20-22	Marrakech Marocco	ECM-23 Satellite Meeting "The enchanting beauty of Moroccan Ornaments" ( <a href="http://www.lcm3b.uhp-nancy.fr/mathcryst/marrakech2007.htm">http://www.lcm3b.uhp-nancy.fr/mathcryst/marrakech2007.htm</a> )	
Aug. 22-27	Marrakech Marocco	ECM-24: European Crystallographic Meeting <a href="http://www.ecm24.org">http://www.ecm24.org</a>	March 30, 2007
Sept. 10-13	Nürnberg Germany	Euromat 2007: Advanced Materials and Processes <a href="http://euromat2007.fems.org">http://euromat2007.fems.org</a>	Jan. 31, 2007
Sept. 10-11	Villigen PSI CH	Annual Meeting of the SGK/SSCr <a href="http://diffraction.web.psi.ch/sgk-sscr-2007.htm">http://diffraction.web.psi.ch/sgk-sscr-2007.htm</a>	June 15, 2007
Sept. 11-12	Villigen PSI CH	User Meeting of the Swiss Light Source <a href="http://www.psi.ch/sls">http://www.psi.ch/sls</a>	to be announced
Oct.7-9	Garmisch Germany	Size-Strain V <a href="http://www.mf.mpg.de/ss-v">http://www.mf.mpg.de/ss-v</a>	Feb. 28, 2007

**2008****Abstract  
Deadline**

May	Gargnano Italy	Summer School on Mathematical and Theoretical Crystallography, <a href="http://www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm">http://www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm</a>	to be announced
May 18-25	Beatenberg CH	IWCGT-4 Fourth International Workshop on Crystal Growth Technology <a href="http://www.beatenberg.ch/IWCGT-4">http://www.beatenberg.ch/IWCGT-4</a>	to be announced
May 31 – June 5	Knoxville USA	Annual Meeting of the American Crystallographic Society <a href="http://www.hwi.buffalo.edu/ACA">www.hwi.buffalo.edu/ACA</a>	to be announced
August Sept. 1-11	Japan Warsaw Poland	IUCR EPDIC-11 European Powder Diffraction Conference	to be announced to be announced
Nov. 17-20	Ghent Belgium	14 <sup>th</sup> International Conference on Thin Films <a href="http://www.ICTF14.UGent.be">http://www.ICTF14.UGent.be</a>	to be announced

**2009**

August	Istanbul Turkey	ECM-25: European Crystallographic Meeting <a href="http://www.ecm25.org">http://www.ecm25.org</a>	to be announced
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**2010**

Sept. 29 – Oct. 5	Darmstadt Germany	ECM-26 and EPDIC-12	to be announced
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## Become a Member of SGK/SSCr

If you are working in the field of crystallography, you will be interested to become a member of our society. For more information as well as online registration, please have a look on our website (<http://www.sgk-sscr.ch>). Presently, the yearly membership fee is sfr. 30 (sfr. 10 for students). For new members, the membership is free until the end of 2006. Please note: SGK/SSCr members can also apply to be a member of the subsection crystal growth (no additional charge) or for individual membership of the European Crystallographic Association, ECA (additional charge: 10 Euro).

**SGK/SSCr is a member of the Swiss Academy of Science.**

<b>Name</b>	
<b>Given name</b>	
<b>Title</b>	
<b>Institution</b>	
<b>Street</b>	
<b>Box/building</b>	
<b>ZIP Code</b>	
<b>Town</b>	
<b>Country</b>	
<b>Phone office</b>	+ ( )
<b>Fax office</b>	+ ( )
<b>Phone private</b>	+ ( )
<b>Mobile phone</b>	+ ( )
<b>E-Mail</b>	@
<b>Interest</b>	
<b>Membership subsection crystal growth</b>	Yes ( ) No ( )
<b>Birth date</b>	Day: Month: Year:
<b>Language(s)</b>	
<b>Major research interests</b>	
<b>Highest degree received</b>	
<b>from university</b>	
<b>Present position</b>	

Date: ..... Place: .....

Signature: .....

**FAX the completed form to: Dr. Radovan Cerny, 022 379.6108**  
**or use our online application form at <http://www.sgk-sscr.ch>**

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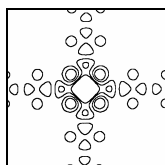
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