

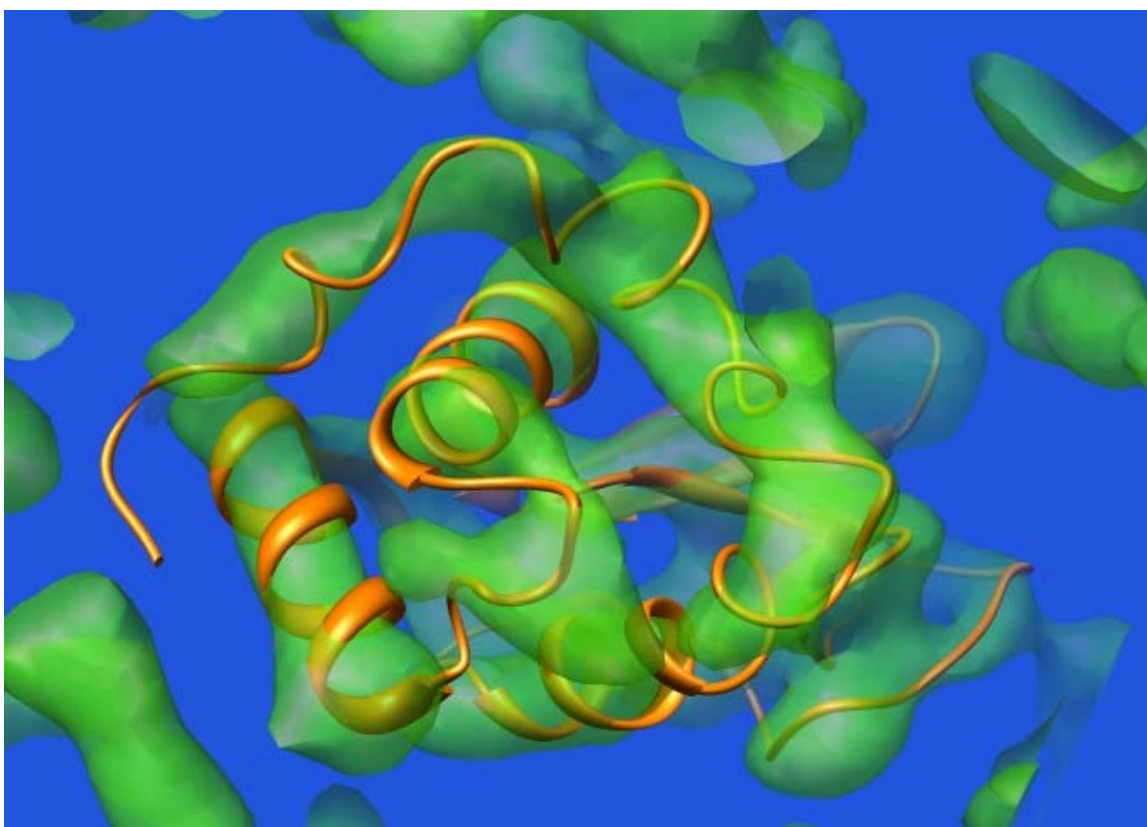


**Schweizerische Gesellschaft für Kristallographie  
Société Suisse de Cristallographie  
Swiss Society for Crystallography**

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

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**SGK/SSCr NEWSLETTER**

**No. 72**

August 2007

In this issue:    Next Generation Instruments for SLS  
                         Annual Meeting of the SGK/SSCr in Villigen, September 12/13, 2007  
                         General Assemblies of the SGK/SSCr and the SKT, September 13, 2007  
                         SLS User Meeting 2007, September 11/12, 2007  
                         Workshop: In-situ experiments at SNBL using high gas pressures

**On the Cover:**

Using powder diffraction for protein structure determination?

The poster abstract "*Experimental phasing of protein powder diffraction data*" by C. Besnard, J. P. Wright, I. Margiolaki, S. Basso, F. Camus, A. N. Fitch, G. Fox, P. Pattison and M. Schiltz shows the details using synchrotron powder diffraction also for proteins (see page 25).

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## Letter from the President

Walter Steurer (steuerer@mat.ethz.ch)

It is summer time, it is the time for conferences, family, research, vacation (listed in alphabetical order). Anyway, whatever you may be doing it is not so easy to forget crystallography and those useful scattering methods. Even when you are just hanging around at a nice place enjoying your cool beer you cannot avoid thinking about bubble sizes, formation frequencies, growth rates, velocities ... multiple scattering of ultrasound<sup>1</sup> will solve the problem, allows you to monitor bubbles in beer, or, equally well, in champagne, if you prefer.

So much for the beer, now to the brains. Forget your *Sudoku*, why don't you try your hand at the definition of a crystal. *What is a crystal?* What a silly question for a crystallographer, you may think, we know that for at least a century, and who cares anyway. However, as the quasicrystallographers know, this question is not so trivial and there is still an ongoing discussion to find a crystal-clear definition<sup>2</sup>.

The discussion started shortly after the discovery of quasicrystals, when the (at that time ad interim) IUCr commission on Aperiodic Crystals tried to find a generalized crystal definition. The old one, based on three-dimensional translational periodicity, obviously did not apply neither to quasicrystals nor to incommensurate structures. For sake of generality, the definition was given in reciprocal space: *by "crystal" is meant any solid having an essentially discrete diffraction diagram, and by "aperiodic crystal" is meant any crystal in which three dimensional lattice periodicity can be considered to be absent.* "Essentially discrete" is a somehow fuzzy term, and, well known to every experimentalist, a diffraction pattern is not really discrete if you consider all the diffraction phenomena originating from real, finite crystals and real radiation sources. Even silicon would not be a crystal following that definition, which is a little bit too pragmatic.

It is summer time, I need a break right now! I see you at our annual meeting, which will take place this year together with the 8<sup>th</sup> SLS User Meeting at PSI, Villigen, September 12-13<sup>3</sup>. Looking forward to seeing you there!

Walter Steurer  
President of the SGK/SSCr

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<sup>1</sup> Physics Today 60 (2007) 49

<sup>2</sup> See <http://www.oldenbourg-wissenschaftsverlag.de/olb/1.c.1163918.de>

<sup>3</sup> <http://user.web.psi.ch/sls07/> and <http://diffraction.web.psi.ch/sgk-sscr-2007.htm>

## Next Generation Instrumentation for SLS

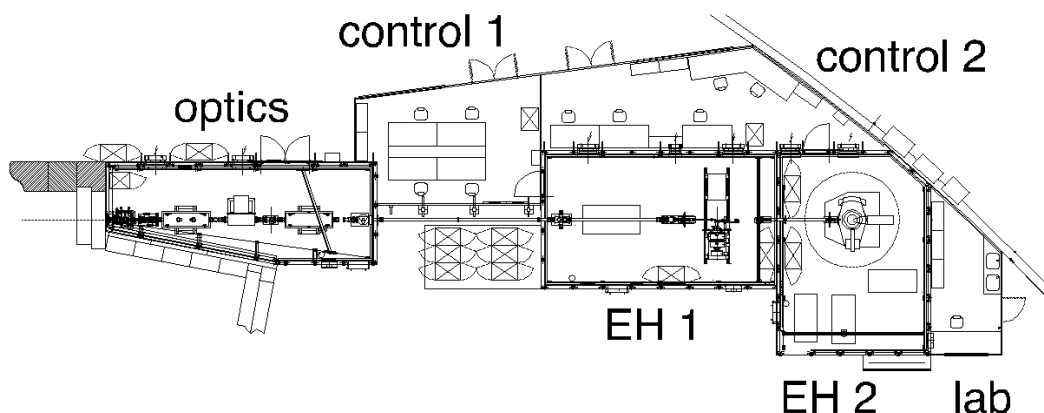
Christoph Quitmann, Laboratory Head LSY II, PSI (christoph.quitmann@psi.ch)  
Jürg Schefer, Head Neutron Diffraction Group, PSI/ETH (Jurg.Schefer@psi.ch)

SLS is starting the planning for the next generation of beam lines to be designed and constructed within 2008 to 2011. Such beamlines can be installed on the remaining bending magnets ports.

Presently, the most interesting instruments for our society are the powder diffractometer at the Materials Science beamline (undulator, 5-40keV, figure 1) and the Protein Crystallography beamlines (PX).

The powder diffractometer (PD) in the experimental hutch EH1 is providing detailed information on the crystallographic structures of materials. It is equipped with two detector systems: A unique microstrip detector covering  $120^\circ$  in  $2\theta$  allows extremely efficient and rapid data collection, an additional crystal analyzer (5 detectors) can be used for very high resolution experiments.

In-situ surface diffraction (SD) is performed in the experimental hutch EH2 using a novel photon-counting 2-D pixel detector (PILATUS 100K) and a five-circle goniometer. Here thin film preparation by pulsed laser ablation is possible in-situ.



**Figure 1:** Layout of the present MS beamline at SLS

The protein crystallography beamlines at the SLS (PXI, II and III) are optimized for very large unit cells, and as a consequence the access is quite restricted to such systems.

In addition the Swiss-Norwegian Beamline at the ESRF is available to Swiss crystallographers. With its two branches it allows high resolution single-crystal diffraction for small molecules and macromolecular crystallography (BM1A) and X-ray Absorption Spectroscopy (XAS) as well as high resolution powder diffraction.

With the option to build further beamlines at the SLS we would like to encourage the members of the SGK/SSCr to submit proposals for a future beamline catering the needs of crystallography. Ideas should be discussed with the division head Friso van der Veen (friso.vanderveen@psi.ch) or the laboratory head Christoph Quitmann (christoph.quitmann@psi.ch). To allow evaluation of competing projects we suggest submitting a 1-2 page project draft detailing the scientific case, the experimental infrastructure necessary and the people involved including their possible contributions to the project. Such drafts should be submitted until March 2008. Decisions of future beamlines will be taken in the second half of 2008 allowing beamline design and installation in 2009 and 2010 respectively. We look forward to discussing interesting plans with you.

## **News for and from Members**

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

Julia Rasch  
(Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, WHGA-343, Villigen PSI, thesis student ILL/PSI)

Dr. Céline Besnard  
(Laboratoire de Cristallographie, EPF Lausanne, BSP 513, SB IMPC LCR2, 1015 Lausanne, Post-Doc)

Dr. Lukas Palatinus (Laboratoire de Cristallographie, EPF Lausanne, BSP 519, SB IMPC LCR2, 1015 Lausanne, Post-Doc)

Fabienne Gschwind (Chemistry Department, University of Fribourg, Chemin du Musée 9, 1700 Fribourg, thesis student)

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

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

- Jean Philippe Rapin (Laboratoire de Cristallographie, Université de Genève)
- Dr. K. Piontek, Institute of Biochemistry, HPMI D8.2, 8093 Zurich

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

## **Travel Grants for Young SGK/SSCr Members**

The committee will award the grants according to the following rules:

- Preference is given to PhD students
- Proof has to be given that there are no grants available covering the expenses
- A supporting letter by the supervisor of the applicant is necessary

If you wish to apply for a travel grant, please send the above mentioned documents to the president of the SGK/SSCr anytime.

At the last board meeting in Bern, June 15, 2007, such a grant was provided to Julia Rasch (PSI/ETHZ/ILL) for participating in the 2007 Zuoz Summer School and to Nicolas Penin (Geneva, for the Gordon Research Conference on "Hydrogen-Metal systems" in Waterville). Reports of their contributions will follow in the next issue of our newsletter.

Details for applications are given at:

<http://www.sgk-sscr.ch/TravelGrants.pdf>

## **New Books**

Kasuku

(contribution by Jacques Deferne, Nora Engel and Alain Gassener)

Texts for beginners and students about crystallography, atoms, minerals and other topics relative to the Planet Earth with PDF-Files available in French.

Ecrits par d'anciens collaborateurs du Muséum de Genève, ces textes scientifiques sont accessibles à tous et vous encouragent à visiter cette Institution où vous trouverez une partie des illustrations.

Nora Engel ([nora.engel@bluewin.ch](mailto:nora.engel@bluewin.ch))

<http://www.kasuku.ch>

## **Pending Membership Fees**

We would like to remind you on the pending membership fees. Your personal balance is always stated on the back of the mailing letter (negative balance: you made a payment for future years)

UBS account: IBAN CH39 0027 9279 C029 1110 0

BIC: UBSWCHZH80A

BLZ: 279

Please avoid cash payments at a post office (PC 80-2-2, UBS Zürich, Account No. 230-C0291110.0) if possible (or add an additional handling fee of CHF 1.20)

Thank you for your cooperation.

Your treasurer,  
Michael Hennig



## Joint Meetings

at

*Paul Scherrer Institut, Villigen, Switzerland*

**CemNet 2007**

**Sept. 10**

**8<sup>th</sup> SLS Users' Meeting**

**Sept. 11/12**

**Annual Meeting 2007 of the  
Swiss Society for Crystallography  
SGK/SSCr and SKT**

**Sept. 12/13**

The Annual Meeting 2007 of the SGK/SSCr/SKT and the 8<sup>th</sup> SLS users' meeting will be organized as a joint meeting **on September 11-13, 2007 at PSI** together with the CemNet 2007 (September 10).

<http://diffraction.web.psi.ch/sgk-sscr-2007.htm>

**Registration:** Deadline: Sept. 5, 2007

The registration is handled by the electronic DUO system of PSI  
(<http://sls.web.psi.ch/goto.php/duo/formhandler.php?DB=18>)

**Dinner September 12, 2007, 19h:** Late registration possible as long as places are available. Please send an E-Mail to:

Jurg.Schefer@PSI.CH (subject= SGK/SSCr/SKT Dinner, September 12, 2007)



## Program of the SGK/SSCr/SKT Meeting and the Joint Session on Direct Methods

The 8<sup>th</sup> SLS User Meeting starts September 11 (day 2), the CEMTEC on September 10 (day 1), see separate programs available from the internet.

	<b>September 12 Wednesday</b>	<b>WLSA/008</b>
<b>14:00 - 14:05</b>	Welcome	P. Willmott, PSI Villigen
<b>14:05 - 14:50</b>	The COBRA method for surface structure determination	Y. Yacoby, Hebrew University, Jerusalem
<b>14:50 - 15:35</b>	Charge flipping - an overview of its use in crystallography	L. Palatinus , EPF Lausanne
<b>15:35 - 16:00</b>	Coffee	
<b>16:00 - 16:45</b>	Reciprocal space phase retrieval methods for reconstructed surfaces	X. Torrelles, CSIO Barcelona
<b>16:45 - 17:30</b>	Solving the phase problem with iterative algorithms	P. Thibault, PSI Villigen
	Concluding remarks	P. Willmott, PSI Villigen
<b>19.00</b>	<b>Dinner SGK/SSCr/SKT</b>	<b>Personalrestaurant OASE, PSI Ost</b>

	<b>September 13 Thursday</b>	<b>WHGA/001</b>
<b>09:00 - 09:05</b>	Welcome to SGK/SSCr Meeting	W. Steurer, ETH Zürich
<b>09:05 - 10:00</b>	The JANA 2006 program package	V. Petricek, Czech Academy of Sciences, Prague
<b>10:00 - 10:50</b>	Structural biology today: Challenges and Examples	F. Winkler, PSI Villigen
<b>10:50 - 11:50</b>	Coffee / poster session	WHGA/001 Lobby
<b>11:50 - 12:15</b>	Appetizer presentations to the poster session	various speakers
<b>12:15 - 14:00</b>	Business Lunch / Poster Session	WHGA/001 Lobby
<b>14:00 - 14:25</b>	Broken symmetries in macromolecular crystals	M. Schiltz, EPF Lausanne
<b>14:25 - 14:40</b>	Synchrotron diffraction to study new forms of light borohydrides	Y. Filinchuk, SNBL/ESRF Grenoble
<b>14:40 - 15:00</b>	Swiss Norwegian beamline: scientific highlights and developments	V. Dmitriev, ESRF Grenoble
<b>15:00 - 15:15</b>	SLS scientific highlights	P. Willmott, PSI Villigen
<b>15:15 - 15:30</b>	SINQ scientific highlights	J. Schefer , PSI Villigen / ETH Zürich
<b>15:30 - 16:30</b>	Coffee / poster session	
<b>16:30 - 17:15</b>	General Assembly of the Swiss Society for Crystallography (SGK/SSCr)	
<b>17:15 - 17:30</b>	General Assembly of the Section Crystal Growth of the SGK/SSCr	

## Abstracts for the SGK/SSCr Annual Meeting 2007

A booklet with all abstracts including the 8<sup>th</sup> SLS User Meeting will be available at the registration desk.



### The program package JANA 2006

V. Petříček<sup>1</sup>, M. Dušek<sup>1</sup> and L. Palatinus<sup>2,1</sup>

<sup>1</sup> Institut of Physics v.v.i., Academy of Sciences of the Czech Republic, Prague

<sup>2</sup> Ecole Polytechnique Fédérale de Lausanne, Laboratoire de Cristallographie, BSP, CH-1015 Lausanne, Switzerland

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Modulated structures manifest themselves by satellite reflections in their diffraction pattern. In order to account for satellites the traditional refinement programs must be modified. The most natural and effective way is based on the superspace theory developed by De Wolff, Janssen & Janner [1], which allows for application of symmetry and generalization of formulas for calculation of structure factors. Thus modulated structures are described by the same set of parameters as in crystallography of standard structures, but the structure parameters (atomic occupancies, coordinates and displacement parameters) are now periodic functions of the actual position of an atom in the crystal. This new periodicity can be generally incommensurate with the basic translation periodicity. The main ideas and several examples of application will be presented in the first part of the lecture.

A non-continuous character of modulation of occupancy has been observed in many structures. A special function called crenel function [2] is to be used for this case instead of harmonic modulation. A new numerical method, based on orthogonalized polynomials has been recently included into the new JANA2006 in order to enhance stability of the refinement. Typical examples illustrate advantages of this approach.

The program Superflip written by L. Palatinus is based on charge flipping [3], a new method for solution of crystal structures. It has been proven to be the best way for the solution of strongly modulated structures. Jana2006 can call directly Superflip and use its results in refinement and interpretation.

Refinement of magnetic structures is a new option in Jana2006. It can be applied even for combination of nuclear and magnetic modulations in the crystal. Another new feature in Jana2006 is the possibility to combine data from different sources. Powder data and single crystal data from neutron as well as X-ray diffraction can be refined simultaneously.

[1] Wolff de P.M., Janssen T. and Janner A. Acta Cryst. **A37**, (1981), 625.

[2] Petříček, V., van der Lee A. & Evain M. Acta Cryst. **A51** (1995), 529.

[3] Palatinus L. Acta Cryst. **A60** (2004), 604.

## Structural biology today: challenges and examples

Fritz K. Winkler, Biomolecular Research, Paul Scherrer Institut, CH-5232 Villigen

E-mail: Fritz.Winkler@psi.ch

Over the past decade instrumental and methodological advances at all levels have made macromolecular crystallography not only much easier and rapid but also permit to tackle more demanding problems. Automation has been introduced in the upfront steps such as protein expression, crystallization and crystal screening as well as in structure determination and these developments are still ongoing. The very large number of structures already known makes it increasingly important to provide new insights into biological function in order to achieve high impact. The combination of low resolution information on large multisubunit systems obtained by electron microscopy or small angle scattering with high resolution structure information of components has proven successful in many cases and illustrates how information at different length scales can provide new information.

Two examples from current projects in our laboratory will be presented. The first addresses key interaction modes of +TIP protein networks which are important for the regulation of microtubule growth which occurs at the positive (+TIP) of these polar cytoskeletal filaments. The second concerns the mechanism and regulation of protein-mediated, facilitated ammonium transport through cell membranes by the integral membrane proteins of the Amt/Rh family.

## Broken symmetries in macromolecular crystallography

M. SCHILTZ

Laboratoire de Cristallographie, *École Polytechnique Fédérale de Lausanne (EPFL)*.

*Marc.Schiltz@epfl.ch*

The space-group symmetry of a crystal structure imposes a point-group symmetry on its diffraction pattern, giving rise to so-called symmetry-equivalent reflections. This introduces a certain redundancy in diffraction data recorded with area detectors and is exploited in macromolecular X-ray crystallography to increase the accuracy of the data by averaging over the symmetry-equivalent measurements (data merging).

Here, we will discuss instances where the symmetry in reciprocal space is broken, *i.e.* where symmetry-related reflections are no longer equivalent. One such situation can occur when the sample suffers from site-specific radiation damage during the X-ray measurement [1,3]. The second example of a broken symmetry is due to the presence of resonant (anomalous) scattering, when the resonant sites display anisotropy in their local atomic environment [2,4,6]. Both situations are common in macromolecular crystallography [5].

In such cases, the genuine intensity differences between symmetry-related reflections can be exploited to yield phase information in the structure solution process. This requires a paradigm shift in the data processing strategy, since the

usual separation of the data merging and phasing steps is abandoned. The data are kept unmerged, down to the Harker construction and the symmetry-breaking effects are explicitly modeled and refined [1,3,6]. Phasing power is generated through the genuine intensity-differences of symmetry-related reflections or repeated measurements of the same reflection recorded at different crystal orientations. Effectively, the operation that is equivalent to data merging is carried out on the complex plane, *i.e.* through the Harker construction: from all the symmetry-related reflections, a single quantity is estimated, but as a complex value ! Since X-ray data in macromolecular crystallography are usually recorded with a certain degree of redundancy, this phase information essentially comes for free.

- [1] M. SCHILTZ, P. DUMAS, C. FLENSBURG, W. PACIOREK, C. VONRHEIN & G. BRICOGNE (2004). Phasing in the presence of severe site-specific radiation damage through dose-dependent modeling of heavy atoms. *Acta Crystallographica D***60**, 78–92.
- [2] G. BRICOGNE, S. C. CAPELLI, G. EVANS, A. MITSCHLER, P. PATTISON, P. ROVERSI & M. SCHILTZ (2005). X-ray absorption, refraction and resonant scattering tensors in selenated protein crystals. Implications for data collection strategies in macromolecular crystallography. *Journal of Applied Crystallography* **38**, 168–182.
- [3] M. SCHILTZ & G. BRICOGNE (2007). Modelling and refining site-specific radiation damage in SAD/MAD phasing. *J. Synchrotron Rad.* **14**, 34–42.
- [4] R. SANISHVILI, C. BESNARD, F. CAMUS, M. FLEURANT, P. PATTISON, G. BRICOGNE & M. SCHILTZ (2007). Polarisation-dependence of anomalous scattering in halogenated DNA and RNA molecules, and importance of crystal orientation in SAD and MAD phasing. *J. Appl. Crystallogr.* **40**, 552–558.
- [5] V. OLIÉRIC, E. ENNIFAR, A. MEENTS, M. FLEURANT, C. BESNARD, P. PATTISON, M. SCHILTZ, C. SCHULZE-BRIESE & P. DUMAS (2007). Using X-ray absorption spectra to monitor specific radiation damage to anomalously scattering atoms in macromolecular crystallography. *Acta Crystallographica D***63**, 759–768.
- [6] M. SCHILTZ & G. BRICOGNE (2007). X-ray polarisation-induced broken symmetries in macromolecular crystals. Submitted.

Yaroslav Filinchuk,<sup>1\*</sup> Aleksandr Talyzin,<sup>2</sup> Hans Hagemann,<sup>3</sup> Dmitry Chernyshov,<sup>1</sup> and Vladimir Dmitriev<sup>1</sup>

<sup>1</sup> Swiss-Norwegian Beam Lines at ESRF, Grenoble, France

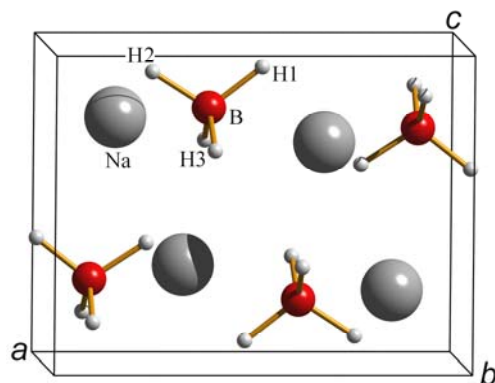
<sup>2</sup> Dpt. of Physics, Umeå University, Sweden

<sup>3</sup> Dpt. of Physical Chemistry, University of Geneva, Switzerland

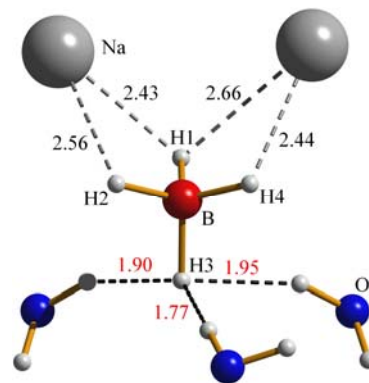
E-Mail: Yaroslav.Filinchuk@esrf.fr

Light metal hydrides are considered as perspective energy carriers for future mobile applications. Hydrogen can be produced from borohydrides of alkaline metals, such as NaBH<sub>4</sub>, by thermal decomposition (pyrolysis) or in a reaction with water (hydrolysis). Interest in structural studies of light borohydrides has increased significantly during recent years. Here we report structures of two new energy-rich forms of NaBH<sub>4</sub>: a high-pressure polymorph of NaBH<sub>4</sub>, which exists above 8 GPa, and the first hydrated borohydride, NaBH<sub>4</sub>·2H<sub>2</sub>O. Both compounds were studied at the Swiss-Norwegian Beam Lines by various synchrotron diffraction techniques.

The ambient pressure fcc  $\alpha$ -phase of NaBH<sub>4</sub> transforms at  $\sim 6$  GPa into a closely related tetragonal  $\beta$ -phase, and above 8 GPa into a new orthorhombic  $\gamma$ -phase [1]. We collected synchrotron powder diffraction data for NaBH<sub>4</sub> in a diamond-anvil cell up to 11.2 GPa. For the successful structure solution, it was absolutely essential to model the sample texture, including it as a variable in a global optimization. Strong texture indicates an oriented growth of crystallites, specific for the  $\beta$ - to  $\gamma$ -NaBH<sub>4</sub> transition. The structure was solved *ab initio* from diffraction data (program FOX) with most crystallites having their *a*-axes approximately aligned with the compression direction, and then refined by the Rietveld method. Elimination of the correction for the preferred orientation leads to an increase in  $R_B$  from 7.9% to 45%. That means that not only the structure solution, but also the refinement would fail if we did not take the texture into account. Elimination of hydrogen atoms increases  $R_B$  from 7.9% to 17%, thus showing that their contribution to X-ray diffraction intensities is sufficient for localization of H-atoms (Figure 1), even from high-pressure synchrotron data.



**Figure 1.** Crystal structure of  $\gamma$ -NaBH<sub>4</sub> at 11.2 GPa, determined *ab-initio* from diamond-anvil cell synchrotron powder diffraction data.



**Figure 2.** Dihydrogen bonds in the coordination environment of the borohydride anion in NaBH<sub>4</sub>·2H<sub>2</sub>O.

The structure of NaBH<sub>4</sub>·2H<sub>2</sub>O was solved from single crystal diffraction data. It contains sodium cations, which are octahedrally coordinated by four water molecules and two borohydride anions. The BH<sub>4</sub><sup>-</sup> anion has a nearly ideal tetrahedral geometry (uncorrected B-H distances 1.110(15)-1.134(13) Å, H-B-H angles 106.8(9)-112.4(10)°) and is bridged with two Na<sup>+</sup> ions via the tetrahedral edges. The structure does not contain classical hydrogen bonds, but reveals strong dihydrogen O-H<sup>δ+</sup>...<sup>δ-</sup>H-B bonds of 1.77-1.95 Å (Figure 2). The H...H distances are much shorter than twice the van der Waals radius of a hydrogen atom (2.4 Å). IR and Raman spectra of NaBH<sub>4</sub>·2H<sub>2</sub>O are consistent with the presence of the dihydrogen bonds for the three O-H groups, and the absence of the dihydrogen bonding for the fourth one.

Synchrotron powder diffraction reveals that within 200-313K the unit cell volume (Å<sup>3</sup>) of NaBH<sub>4</sub>·2H<sub>2</sub>O increases linearly with temperature (K):  $V = 825.3(1) + 0.1969(4) T$ . The structure decomposes at 313-315K into NaBH<sub>4</sub> and H<sub>2</sub>O. The resulting products react, releasing hydrogen.

These case studies [2, 3] illustrate the ability of synchrotron diffraction techniques to characterize in detail light hydrides modified by pressure or chemical composition.

- [1] R. S. Kumar, A. L. Cornelius, Appl. Phys. Lett. **87**, 261916 (2005).
- [2] Y. Filinchuk, A. Talyzin, D. Chernyshov, V. Dmitriev, Phys. Rev. B, accepted.

#### Scientific highlights and new developments at SNBL

V. Dmitriev  
Swiss-Norwegian Beam Lines at ESRF, Grenoble, France

E-Mail: dmitriev@esrf.fr

Events and improvements on the Swiss-Norwegian beam-lines (SNBL) will be presented in the talk. Significant progress in instrumentation development made over the last months, new instruments and sample environment devices will be demonstrated on a selection of some experiments carried out by our users. Upcoming developments will be exposed.

#### Status report and new developments at the SLS

Phil Willmott  
Materials Science Beamline, SLS

E-Mail: philip.willmott@psi.ch

Beamline development and milestones at the SLS will be presented, in particular with reference to hard x-rays and diffraction. A small selection of scientific highlights will also be presented from the Materials Science beamline and other stations.

J. Schefer Laboratory for Neutron Scattering, ETHZ & PSI, 5232 Villigen  
Jurg.Schefer@PSI.CH

We present the status of the instrumentation operated by the Laboratory for Neutron Scattering, ETHZ&PSI - focusing on diffraction instruments – as well as scientific highlights from the past years. Special attention will be given to new instruments under commissioning and development.

## Posters

### Small molecule crystallography at the SLS X06SA Beamline

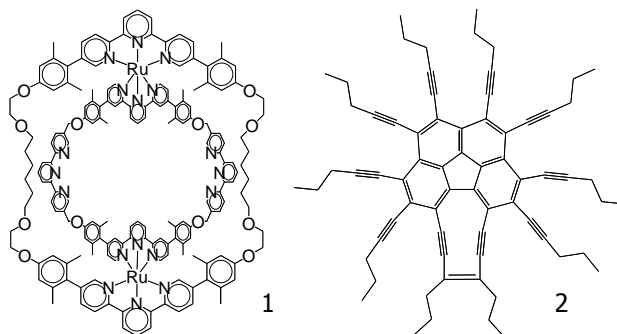
A. Linden<sup>1</sup>, M. Wang<sup>2</sup>, H.-B. Bürgi<sup>1</sup> and C. Schulze-Briese<sup>2</sup>

<sup>1</sup> Institute of Organic Chemistry, University of Zürich

<sup>2</sup> SLS, Paul Scherrer Institute, Villigen

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The group of Prof. Jay Siegel at the OCI of the University of Zürich is synthesising small molecules, like **1** (Jeremy Klosterman) and **2** (Tomoharu Hayama), which have topologies that lend themselves to heavily disordered or solvated structures and, consequently, weak diffraction or even diffuse scattering. No useable data could



be collected from large crystals of **1** and **2** on the OCI's in-house Nonius *KappaCCD* diffractometer, so we turned to a synchrotron source.

The X06SA beamline at the SLS is designed for protein crystallography and has a Mar225 CCD detector with a single circle ( $\phi$ ) goniometer and a minimum crystal-detector distance of 80 mm. The beamline delivers  $10^{12}$  photons/sec (total flux) to the crystal in a well collimated and focused way, resulting in a beam which is 50 million times brighter than normal laboratory X-ray source. To test the utility of this facility for small molecule work, we collected data from four test crystals of small organic and metal-organic molecules, which had previously given excellent structural

results on the in-house diffractometer. Full data sets could be collected to a resolution limit of about 0.8 Å in about 10 minutes with high beam attenuation at wavelength of 0.71 Å. The refinement results were of the same high quality as with the in-house data. The one drawback is the low completeness of the unique reflections (as low as 67% in one case), which is a consequence of the long minimum crystal-detector distance and the single circle goniometer. This limitation will be overcome with the installation of a Kappa Goniometer in 2008.

The synchrotron data for **1** allowed the structure to be solved, which confirmed the expected compound, but a high *R*-factor (0.24) remained. It is suspected that the crystals are not true single crystals, but their intense color prevented proper visual inspection. The structure of **2** could also be solved only from the synchrotron data and yielded *R* = 0.12. There are three planar molecules in the asymmetric unit and each is potentially 10-fold disordered, hence the weak diffraction and diffuse scattering. Difference *Fourier* maps revealed at least 8 main orientations among the three molecules and refinement required 5049 parameters and 28418 restraints! The structure geometry, despite the disorder, agrees very well with that calculated theoretically. The structures of **1** and **2** could only be determined at all because of the availability of the synchrotron radiation.

#### Magnesium borohydride : synthesis and crystal structure

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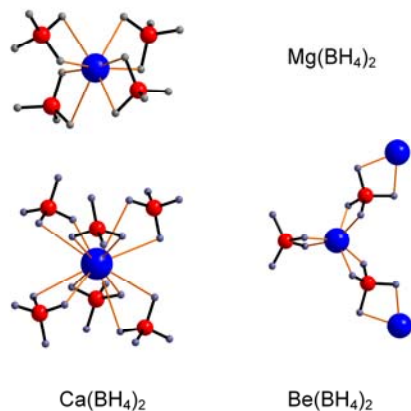
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<http://dx.doi.org/10.1002/anie.200700773>

Magnesium borohydride (Mg(BH<sub>4</sub>)<sub>2</sub>), which has been known since the 1950s [1], has a theoretical hydrogen storage capacity of 14.8 wt%. No structural data were reported, owing to difficulties in obtaining crystalline products of sufficient quality for diffraction methods.

Herein, we present the room temperature crystal structure and Raman spectrum of solvent-free Mg(BH<sub>4</sub>)<sub>2</sub>. The compound was synthesized by the metathesis reaction of LiBH<sub>4</sub> and MgCl<sub>2</sub> in diethyl ether. Its structure was solved (program FOX [2]) from synchrotron (SNBL) and neutron (SINQ) powder diffraction data. In contrast to theoretical predictions, the structure has hexagonal symmetry (*a* = 10.3182(1), *c* = 36.9983(5) Å, *P*6<sub>1</sub>), and contains five symmetry-independent Mg<sup>2+</sup> ions and ten symmetry-independent [BH<sub>4</sub>]<sup>-</sup> ions. The structure was refined jointly on both data by using TOPAS Academic [3]. The BH<sub>4</sub> tetrahedra were kept as semirigid bodies with ideal tetrahedral bond angles and a common refined B-H distance.

Each  $[\text{BH}_4]^-$  ion is approximately linearly coordinated by two  $\text{Mg}^{2+}$  ions. Each  $\text{Mg}^{2+}$  ion is surrounded by four  $[\text{BH}_4]$  tetrahedra arranged in a deformed tetrahedron, resulting in an unusual eightfold hydrogen coordination environment.



The structure of  $\text{Mg}(\text{BH}_4)_2$  differs from those of its beryllium and calcium analogues, as well as from those predicted by theory.

The structure is one of the most complex atom arrangements solved from powder diffraction data so far.

**Figure 1.** Structural comparison of the  $\text{M}(\text{BH}_4)_2$  series' members, M (in blue) = Mg and Ca: 3-d framework; Be: 1-d polymer. Coordination of Mg5 is shown for  $\text{Mg}(\text{BH}_4)_2$ .

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### Magnetic properties of the 2D intercalated disulfide $\text{CuCrS}_2$

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Due to the features of their crystal structure, quasi two-dimensional layered substances can be of great interest for new multilayer thin-film structures. Intercalation and cation substitution allow the tuning of the electronic and magnetic properties such as the colossal magnetoresistance (CMR) effect. Layered transition metal dichalcogenides exhibit a three dimensional crystal structure with strong

anisotropy of the chemical bonds in  $c$  direction, perpendicular to the layers. Whether this crystallographic peculiarity is interrelated with the magnetic properties is the subject of our present investigations.

According to the classification of layered disulfides of  $3d$  metals created by Wilson and Yoffe [1]  $\text{CuCrS}_2$  is an intercalated compound based on the chromium disulfide  $\text{CrS}_2$  with space group  $R\bar{3}m$ . In contrast to related isostructural compounds  $\text{NaCrSe}_2$ ,  $\text{AgCrSe}_2$  and  $\text{NaCrS}_2$ , which all have positive Curie-Weiss temperatures [2],  $\text{CuCrS}_2$  shows a large negative Curie-Weiss temperature of  $\Theta_p = -148$  K [3]. The magnetic structure of  $\text{NaCrSe}_2$  was found to be commensurate, while  $\text{AgCrSe}_2$  and  $\text{NaCrS}_2$  form helices with rotating moments in the basal plane. For the more complex system  $\text{CuCrS}_2$ , earlier neutron diffraction experiments discovered also a helical magnetic propagation vector [4], which could be confirmed with our powder but not with single crystal measurements. Another related compound  $\text{LaCrS}_3$  features complex magnetic properties which are reminiscent of spinglass behavior [5]. The reason is a two-dimensional triangular distribution of  $\text{Cr}^{3+}$  ions in which antiferromagnetic coupling leads to topological frustration. The chromium framework is also a characteristic in our compound  $\text{CuCrS}_2$ .

First results on  $\text{CuCrS}_2$  obtained with powder and single crystal diffraction experiments are presented, supplemented with susceptibility and magnetization measurements. They should contribute to a better understanding of the magnetic structure of  $\text{CuCrS}_2$ .

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## Crystal structure of the human Pim-2 Kinase in complex with a Ruthenium organometallic inhibitor

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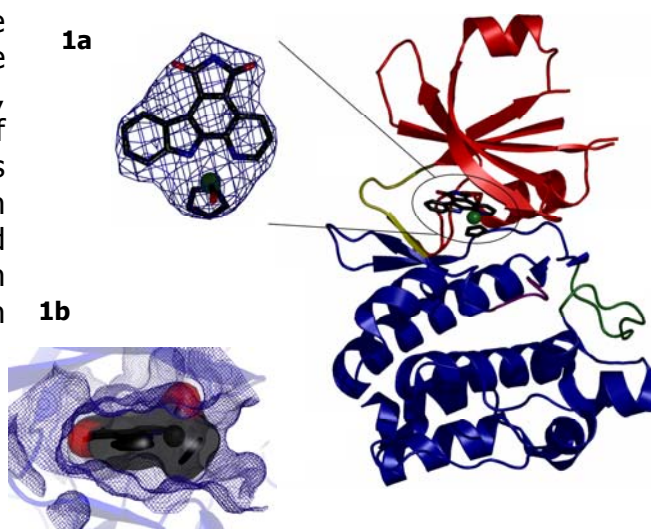
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The Pim kinases are a family of three vertebrate protein serine/threonine kinases (Pim-1, Pim-2, and Pim-3), which are critical for the regulation of a variety of cellular functions including cell growth, proliferation and survival [1]. Especially Pim-1 and Pim-2 play an important role in cytokine signaling pathways in hematopoietic cells and are implicated in the development of a number of leukemia's and solid tumors [2,3]. Recent data suggest that Pim-2 may be responsible for resistance of leukemia cells to the cancer drug rapamycin [4]. This makes Pim-2 a major target for cancer therapy. Strong and specific inhibitors are sought in order to block the activity of Pim-2 and so terminate tumor growth.



We solved the crystal structure of Pim-2 in complex with a strong and potentially selective inhibitor to 2.7 Å resolution. The rigid ruthenium half-sandwich complex binds in the active site between the N-terminal and the C-terminal domain (**1a**). It fits tightly into the binding pocket showing a very nice shape complementarity (**1b**). *In-vivo* studies in tumor cells will show if this compound can be used as a drug for cancer therapy.

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Here we present for the first time resonant soft x-ray powder diffraction data and successfully observe the magnetic reflection ( $1/2\ 0\ 1/2$ ) in the  $RNiO_3$  family [1] at the Ni  $L_{2,3}$  edges and the orbital reflection ( $1/4\ 1/4\ 0$ ) at the Mn  $L_{2,3}$  edges in the half doped manganate system  $RBaMn_2O_6$  (R=rare earth ion). Polarization, temperature and energy dependence of the ( $1/2\ 0\ 1/2$ ) powder diffraction peak prove the magnetic origin of the scattered signal. The advantage of resonant soft x-ray powder diffraction against neutron powder diffraction is exemplified by the sensitivity to the electronic states. Here we present the energy dependence versus metal-insulator transition temperatures (or versus ionic size of the R ions). The ( $1/4\ 1/4\ 0$ ) reflection in half doped manganates directly probes the orbital order of the  $Mn^{3+}$  sites. The energy dependence of the reflection in comparison with other half doped manganates gives clear evidence that these manganates have all the same type of orbital ordering. The temperature dependence of the R=Sm compound shows a strong increase in intensity at approximately 200K, which gives direct evidence of a rearrangement of the orbital stacking along the c axis, keeping the in plane orbital order unaffected. These results prove that resonant x-ray scattering can be performed even on polycrystalline materials in the soft x-ray regime due to the very large enhancement factors at these edges. This allows us to directly probe ordering phenomena in the valence shell of transition metal elements in relatively simple way.

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Gap opening through charge disproportionation in RNiO<sub>3</sub> perovskites:  
New neutron diffraction and x-ray absorption results

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With the exception of metallic LaNiO<sub>3</sub>, all the members of the RNiO<sub>3</sub> series (R = rare earth or Y) undergo a sharp metal to insulator transition at transition temperatures  $T_{MI}$  ranging between 130K (Pr) and 600K (Lu). The mechanism of the gap opening is not yet fully understood and has been a matter of controversy since its discovery in 1991. Recently, the existence of a symmetry decrease from orthorhombic Pbnm to monoclinic P2<sub>1</sub>/n at  $T_{MI}$  was reported for the last members of the series (Ho to Lu) and interpreted as signature of an incomplete  $2Ni^{3+} + Ni^{3+\delta} + Ni^{3-\delta}$  charge disproportionation (CD) with  $\delta = 0.3$ . [1] This mechanism provides a new framework for the M-I transition and, due to the diamagnetic nature of Ni<sup>4+</sup>, could also account for the unusual magnetic structure displayed by these compounds. However, due to the smallness of the structural changes associated to the CD, no experimental evidence of this phenomenon could be found to date for the first members of the series (Pr to Dy).

In this study we report new, combined ultra-high resolution powder neutron diffraction and x-ray absorption measurements on the full RNiO<sub>3</sub> series, as well as high-pressure neutron diffraction data on PrNiO<sub>3</sub>. In contrast with previous studies, we observe a nearly complete charge disproportionation for the nickelates with small rare earths, as well as a progressive evolution towards a non-disproportionated state moving from Lu ( $\delta = 1$ ) to Pr ( $\delta = 0.2$ ).

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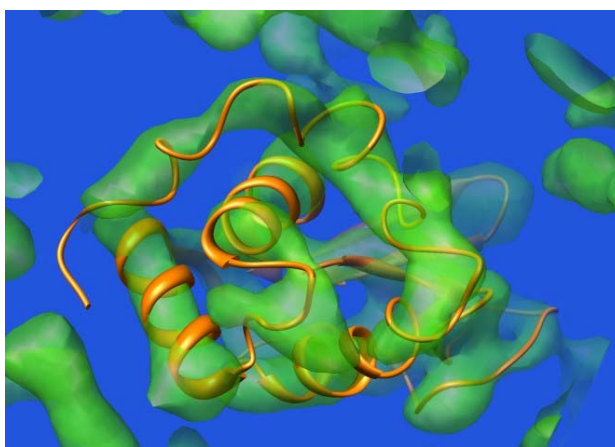
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The preparation of single crystals suitable for x-ray analysis is frequently the most difficult step in structural studies of proteins. With the aid of two examples, it is shown that de novo solution of the crystallographic phase problem can be achieved at low resolution using microcrystalline powder samples via the isomorphous replacement method. With synchrotron radiation and optimized instrumentation, high-quality powder patterns have been



recorded, from which it was possible to generate phase information for structure factors up to 6 Å resolution. pH- and radiation-induced anisotropic lattice changes were exploited to reduce the problem of overlapping reflections, which is a major challenge in protein powder diffraction. Using the Single Isomorphous Replacement method, the resulting data are of sufficient quality to compute molecular envelopes of the protein molecule and to map out the solvent channels in the crystals, which are essential structural data for the characterization of microcrystalline proteins as novel mesoporous materials. A further step is achieved by using the Multiple Isomorphous Replacement method, since the density maps obtained are of sufficient quality to start assigning the secondary structure elements of the protein.

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The intense X-ray fluxes associated with third generation synchrotron sources can result in significant damage to cryo-cooled macromolecular crystals [1-4]. For brominated compounds, even a relatively moderate X-ray dose can induce sufficient debromination to prevent structure determination [3]. However, specific X-ray damage can provide additional phase information, ultimately allowing to determine a protein structure using a single crystal from a native macromolecule [2, 4].

In the present study [5], we show that a series of absorption spectra recorded on a brominated RNA faithfully monitor the extent of C-Br bonds cleavage. Modification of the fluorescence spectrum correlates well with the cumulated X-ray dose and these measurements help to follow the radiation-induced debromination event. This will be useful for standard SAD/MAD experiments and for the emerging 'Radiation damage Induced Phasing' method exploiting both the anomalous signal of an anomalous scatterer and the 'isomorphous' signal resulting from the cleavage.

In addition, we have made striking verifications of the influence of crystal orientation relative to the beam polarization on the height of a 'white line' (*i.e.* on the value of  $f''$ ). Depending on the crystal orientation, the 'white line' can disappear completely. Thus, the correct choice of sample orientation allows to optimize the anomalous signal and can be crucial for a successful structure determination [6].

These results are not limited to bromine and can be extended to any element having an absorption edge in the commonly available wavelength/energy range.

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Laue diffraction has for a long time been used for determination of crystal quality due to its sensitivity to defect content and defect arrangement. Through the development of suitable focusing optics revival of the white beam diffraction has emerged into micro diffraction techniques with beam sizes down to the micron and even sub-micron range. In our work Laue micro diffraction has been performed on single crystal gold micron pillars at the mXAS beam line of the Swiss Light Source (SLS). At the same time the crystal is strained. Micro compression of single crystal micron pillars has gained considerable interest since it was shown that fcc metals exhibit an increase of the pillar strength with decreasing diameter. However variations of deformation mode and differences in the stress-strain behavior have been reported. Therefore we combine the micro compression technique with micro focused Laue diffraction experiments, which allows capturing changes in microstructure and defect structure as a function of time.

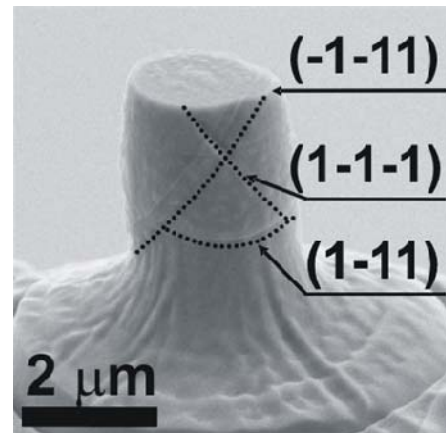


Fig. 1: Electron Microscopy evidences three active slip planes during compression.

This makes it for the first time possible to follow the evolution of Laue diffraction peaks during micro pillar deformation and establish their direct relation to the obtained stress-strain-data from micro compression of Au micron sized pillars. At odds to what was previously assumed our results demonstrate the existence of pre-existing strain gradients that are believed to strongly promote plasticity on hard slip systems for smaller pillars (see figure 1), whereas for the larger pillars classically predicted deformation via slip is observed [1,2]. Furthermore the presented work evidences for the first time crystal rotation of the strained micro pillars, which is ascribed to the complex geometrical boundary conditions of the experimental technique. Our results underline the importance of performing micromechanical testing in-situ to reveal the dynamics of small scale plasticity of these new testing techniques.

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## The (3+1) Dimensional Scheelite Structure Type

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The incommensurately modulated scheelite-like structure  $\text{KNd}(\text{MoO}_4)_2$  [1] (superspace group  $I2/b(\alpha\beta 0)00$ ;  $a = 5.5202(2)$ ,  $b = 5.33376(5)$ ,  $c = 11.8977(3)$  Å,  $\gamma = 90.9591(7)^\circ$ ,  $\mathbf{q} = 0.57789(4)\mathbf{a}^* - 0.14748(6)\mathbf{b}^*$ ; two building units,  $A = (\text{K}, \text{Nd})$  in [ $4e$ :  $1/2 \ 1/4 \ z \approx 0.88$ ] and  $X = [\text{MoO}_4]$  in [ $4e$ :  $1/2 \ 1/4 \ z \approx 0.38$ ]) has been exploited as a natural (3+1)D superspace model to generate a large portion of the scheelite-like 3D structure family. Although each member differs in space group symmetry, unit cell parameters and composition, in (3+1)D space however, they share a common superspace group, a common number of building units in the basic unit cell occupying Wyckoff sites with specific coordinates ( $x, y, z$ ) and specific basic unit cell axial ratios ( $c/a, a/b, b/c$ ) and angles. Variations of the modulation vector  $\mathbf{q}$ , occupation functions and  $t_0$  are exploited for the derivation. Eight topologically and compositionally different known structures ( $\text{RbBi}[\text{MoO}_4]_2$ ,  $\text{K}_2\text{Th}[\text{MoO}_4]_3$ ,  $\text{Eu}_2[\text{WO}_4]_3$ ,  $\text{Bi}_2[\text{MoO}_4]_3$ ,  $\text{La}_2[\text{MoO}_4]_3$ ,  $\text{Bi}_3[(\text{FeO}_4)(\text{MoO}_4)_2]$ ,  $\text{Na}_4\text{Zr}[(\text{MoO}_4)_4]$ ,  $\text{Na}_4\text{Y}[\text{Na}'(\text{MoO}_4)_4]$ ) are compared with their models derived from the  $\text{KNd}(\text{MoO}_4)_2$  structure in order to evaluate the capabilities and limitations of the incommensurately modulated structure as a superspace generating model. Applications of the  $\text{KNd}(\text{MoO}_4)_2$  structure as a starting model for the refinement of  $\text{KSm}(\text{MoO}_4)_2$  [2] and the prediction of  $\text{KEu}(\text{MoO}_4)_2$  [1] and  $\text{KLa}(\text{MoO}_4)_2$  [2] modulated members of the family are also shown. This family can be considered as the (3+1) dimension scheelite structure type. The presentation of the scheelite-like structures as members of the (3+1) dimension scheelite structure type reveals new structural relations, which remain hidden if only conventional 3D structure descriptions are applied.

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Metal-Peptide Frameworks: combining self-assembling properties of small peptides and metal coordination chemistry to create new Metal-Organic frameworks structures

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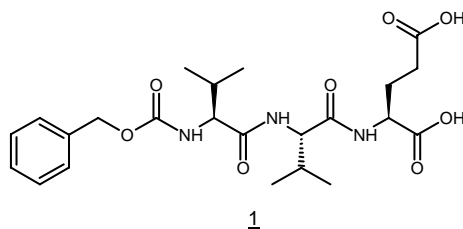
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<sup>4</sup> A. Taubert, Institute of Chemistry, University of Potsdam, D-14476 Golm and Max-Planck-Institute of Colloids and Interfaces, D-14476 Golm, Germany

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Chiral Metal Organic Frameworks<sup>[1],[2]</sup> are currently subject of intense research for their applications in asymmetric catalysis, chiral separation, adsorption-release, filtrations and in all cases a chiral structure would be of advantage. Exploring the rules to synthesize these new smart and responsive materials is of interest. To that respect, small self-assembling peptides would be excellent candidates as ligands because of their chemical variety, chiral information and (relative) flexibility.

In this context, and continuing our efforts to use small self-assembling peptides to organize nanoparticles or to template inorganic material-based nanostructures<sup>[3]</sup>, we designed a small peptide of formula Z-Val-Val-Glu(OH)OH (structure given figure 1) which can self-assemble under the influence of metal ions like copper (II). We describe here the crystallographic characterization of the complex prepared from 1 and copper (II) in ammoniacal conditions.



**Figure 1:** Structure of the peptide used

As the complex was only formed as a powder, we thus used *ab initio* crystal structure solution from synchrotron powder diffraction data. Using Fox software<sup>[4]</sup> and all the chemical information gained by different spectroscopic methods (SQUID, EPR, FT-IR...) we were able to generate a structure compatible with the powder X-Ray information. The peptide-copper complex self-assembles in  $\beta$  sheets and presents porosity which can be used to store small molecules or gases. This first

model is a good candidate for the further design of more complex Metal-Peptides Frameworks and is a good proof of the applicability of Fox to solve large structures.

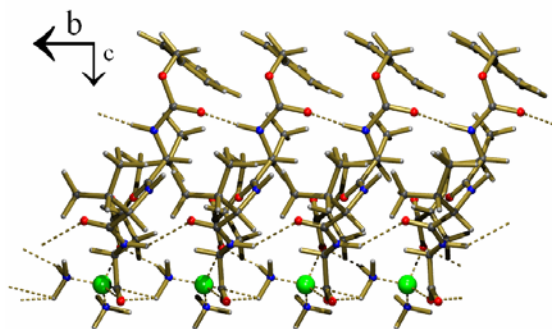


Figure 2:  $\beta$  sheet structure adopted by the complex

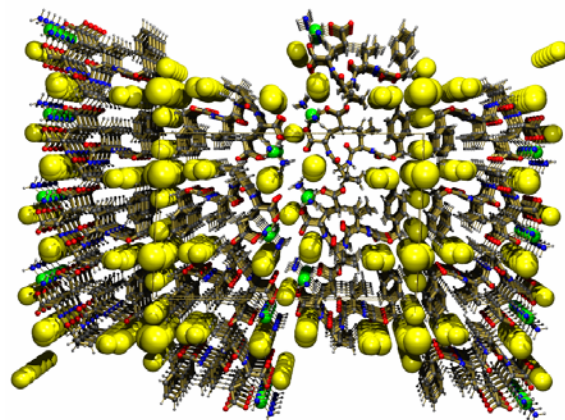


Figure 3: Packing scheme of the MPF-9 showing porous structure (grey balls)

- [1] Rowsell, J. L. C. , Yaghi, O. M., *Micro. Meso.*, **2004**, *73*, 3-14
- [2] Kesanli, B., Lin, W., *Coord. Chem. Rev.*, **2003**, *246*, 305-326
- [3] Manton, A., Taubert, A., *Macromolecular Bioscience*, **2007**, *7*, 208-217
- [4] Favre-Nicolin, V., Cerny, R., *J. Appl. Cryst.*, **2002**, *35*, 734-743  
Software available at <http://objcryst.sourceforge.net>.

## Agenda of the SGK/SSCr General Assembly 2007

September 13, 2007, Villigen PSI, WHGA/001, 16.30h



- a) Jahresbericht/le rapport annuel
- b) Jahresrechnung/les comptes annuels
- c) Aufstellung des Budgets für das kommende Jahr/le budget proposé pour l'année suivante
- d) Festsetzung des jährlichen Mitgliederbeitrages/le montant de la cotisation annuelle
- e) Notwendige Wahlen (Wahl des Vorstandes gemäß Art. 16, zweier Rechnungsrevisoren, des Delegierten in den Senat der SANW und dessen Stellvertreter. Alle müssen Mitglieder der SGK sein)
- e) les élections statutaires (élection du comité selon l'art. 16, nomination des deux réviseurs de comptes, du délégué et de son représentant au sénat de l'ASSN. Tous doivent être membre de la SSCr.
- f) Eventuelle Statutenänderungen/les modifications éventuelles des statuts  
The board has prepared a proposal for a change in the by-laws, as asked by the last assembly 2006 in Bern. The proposal is attached below.
- g) Anträge von Mitgliedern

## Amendments of the by-laws of the Swiss Society for Crystallography (SGK/SSCr)

The committee of the SGK/SSCr suggests a few amendments of the by-laws of the SGK/SSCr in order to take the continuously changing structure and self-understanding of our society into account. Likewise as the official version (see [http://www.sgk-sscr.ch/Statuts\\_SSCr.html](http://www.sgk-sscr.ch/Statuts_SSCr.html)), the suggested amendments are formulated in German and will be translated after the acceptance by the general assembly.

	<i>old</i>		<i>new</i>
<b>Art. 1</b>	<p><i>Er macht es sich zur Aufgabe, die Kristallographie (Kristallmathematik, Kristallphysik [inklusive Kristallwachstum und Kristallzüchtung], Kristallchemie und Kristallstrukturbestimmung), den persönlichen Kontakt ihrer Mitglieder in der Schweiz und die Beziehungen zur Schweizerischen Mineralogisch-Petrographischen Gesellschaft (SMPG), Schweizerischen Chemischen Gesellschaft (SchG), Schweizerischen Physikalischen Gesellschaft (SPG) sowie zu ausländischen kristallographischen Assoziationen, Gesellschaften, Sektionen oder internationalen Vereinigungen (z.B. International Union of Crystallography [IUCr], International Organization of Crystal Growth [IOCG]), an deren Versammlungen sich die SGK vertreten lassen kann, zu pflegen.</i></p> <p><i>Dabei soll besonderer Wert darauf gelegt werden, die verschiedenen kristallographischen Forschungsrichtungen in Chemie, Kristallographie, Physik und Technik einander näher zu bringen.</i></p>	<p>wird ersetzt durch</p> <p>wird ersetzt durch</p>	<p><i>Er macht es sich zur Aufgabe, die Kristallographie in allen ihren Aspekten zu fördern und die Beziehungen zu verwandten Wissenschaftsgebieten und deren Gesellschaften zu pflegen. Dazu zählen insbesondere die Schweizerische Chemische Gesellschaft (SCHG), Schweizerische Mineralogisch-Petrographische Gesellschaft (SMPG), Schweizerische Physikalische Gesellschaft (SPG) sowie ausländische kristallographische Gesellschaften und internationale Vereinigungen wie die International Union of Crystallography (IUCr) und der International Organisation for Crystal Growth (IOCG).</i></p> <p><i>Dabei soll besonderer Wert darauf gelegt werden, die verschiedenen kristallographischen Forschungsrichtungen in Biologie, Chemie, Kristallographie, Materialwissenschaft, Physik und Technik einander näher zu bringen.</i></p>
<b>Art. 2</b>	<p><i>Diejenigen Mitglieder der SGK, welche sich besonders</i></p>	<p>wird</p>	<p><i>Mitglieder der SGK, die eine feste Organisationsstruktur für die För-</i></p>

	<i>für die Probleme des Wachstums von Kristallen und epitaktischen Schichten sowie für Kristallzüchtung und Kristallbearbeitung interessieren, vereinigen sich in einer "Sektion für Kristallwachstum und Kristalltechnologie (SKT)", Section de Croissance et Technologie des Cristaux (SCT), Section for Crystal Growth and Crystal Technology (SCT).</i>	ersetzt durch	<i>derung ihrer speziellen Interessensgebiete wünschen, können sich in Sektionen organisieren. Diejenigen Mitglieder der SGK, welche sich besonders für die Probleme des Wachstums von Kristallen und epitaktischen Schichten sowie für Kristallzüchtung und Kristallbearbeitung interessieren, vereinigen sich in einer "Sektion für Kristallwachstum und Kristalltechnologie (SKT)", Section de Croissance et Technologie des Cristaux (SCT), Section for Crystal Growth and Crystal Technology (SCT).</i>
<b>Art. 5</b>	<i>Die SGK besteht aus persönlichen und unpersönlichen Mitgliedern, sowie aus Ehrenmitgliedern. Jedermann, der sich für Kristallographie (inklusive Kristallwachstum und Materialforschung) interessiert, kann die Mitgliedschaft beantragen; über die Mitgliederaufnahme entscheidet der Vorstand.</i>	wird ersetzt durch	<i>Die SGK besteht aus persönlichen und unpersönlichen Mitgliedern, sowie aus Ehrenmitgliedern. Alle, die sich für Kristallographie interessieren, können die Mitgliedschaft beantragen; über die Aufnahme von Mitgliedern entscheidet der Vorstand</i>
<b>Art 6</b>	<i>Die persönlichen Mitglieder entrichten einen jährlichen, durch die Mitgliederversammlung bestimmten, Mitgliedsbeitrag. Die SKT kann einen Sektionsmitgliedsbeitrag erheben. Jahresbeiträge sind zu Beginn des laufenden Jahres fällig. Das Vereinsjahr ist das Kalenderjahr.</i>	wird ersetzt durch	<i>Die persönlichen Mitglieder entrichten einen jährlichen, durch die Mitgliederversammlung bestimmten, Mitgliedsbeitrag. Jahresbeiträge sind zu Beginn des laufenden Jahres fällig. Das Vereinsjahr ist das Kalenderjahr.</i>
<b>Art 16</b>	<i>Der Vorstand setzt sich aus dem Präsidenten, dem Vizepräsidenten, dem Sekretär-Kassier (Aktuar) und drei Beisitzern zusammen.</i>	wird ersetzt durch	<i>Der Vorstand setzt sich aus dem/der Präsidenten/in, dem/der Vizepräsidenten/in, dem/der Sekretär/in, Kassier/in und zwei Beisitzern/Beisitzerinnen zusammen.</i>
	<i>Die SKT wählt eine Sektions-</i>		<i>Jede Sektion wählt eine Sektions-</i>

*leitung, bestehend aus einem oder zwei Vorsitzenden, einem Sekretär, einem Kassier und 2 - 4 Beisitzern für die Dauer von drei Jahren*

wird  
ersetzt  
durch

*leitung bestehend aus einem/einerer Sektionsleiter/in und einem/einer Sektionssekretär/in für die Dauer von drei Jahren.*

## **Art 17**

*Der Vorstand wählt aus seiner Mitte den Sekretär für die IUCr, zwei Delegierte an jede General Assembly der IUCr (verbunden mit Internationalem Kristallographenkongress) sowie Delegierte an eventuelle weitere Körperschaften (diese letzteren brauchen nicht dem Vorstand anzugehören). Die Amtsdauer des Sekretärs für die IUCr beträgt sechs Jahre; er besorgt den Verkehr mit der IUCr und ist der eine Delegierte. Er wird jeweils für zwei aufeinanderfolgende General Assemblies, der zweite Delegierte nach Uebereinkunft gewählt. Der Präsident der SGK ist gleichzeitig Vorsitzender des Schweizerischen Komitees für die IUCr. Der Sektionsleiter der SKT ist gleichzeitig der Vorsitzende des Schweizerischen Komitees und Delegierter im IOCG; der zweite Delegierte ist sein Sekretär.*

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durch

*Der Vorstand wählt aus seiner Mitte den/die Sekretär/in für die IUCr, zwei Delegierte an jede General Assembly der IUCr, sowie Delegierte an eventuelle weitere Körperschaften (diese letzteren brauchen nicht dem Vorstand anzugehören). Die Amtsdauer des/der Sekretärs/Sekretärin für die IUCr beträgt sechs Jahre; er/sie besorgt den Verkehr mit der IUCr und ist der/die eine Delegierte. Er/Sie wird jeweils für zwei aufeinanderfolgende General Assemblies, der/die zweite Delegierte nach Uebereinkunft gewählt. Der/Die Präsident/in der SGK ist gleichzeitig Vorsitzende/r des Schweizerischen Komitees für die IUCr. Sektionsleiter/in und sein/ihr/e Stellvertreter/in der SKT ist gleichzeitig der/die Vorsitzende des Schweizerischen Komitees und Delegierte/r im IOCG; der/die zweite Delegierte im IOCG ist der/die Sektionssekretär/in der SKT.*

*Gehören Delegierte nicht dem Vorstände an, so können sie mit beratender Stimme zu den Vorstandssitzungen beigezogen werden. Präsident und Sekretär führen die für die SGK verbindliche, rechtsgültige Unterschrift; Präsident oder Vizepräsident und Sektionsleiter diejenige für die SKT.*

wird  
ersetzt  
durch

*Gehören Delegierte nicht dem Vorstände an, so können sie mit beratender Stimme zu den Vorstandssitzungen beigezogen werden. Präsident und Sekretär führen die für die SGK verbindliche, rechtsgültige Unterschrift; Präsident oder Vizepräsident und Sektionsleiter diejenige für die Sektionen.*

## **1<sup>st</sup> Announcement of a Workshop on**

### **In-situ experiments at SNBL using high gas pressures**

Grenoble on 8-9 November 2007

Contact: philip.pattison@epfl.ch

A proper understanding of structure-property relationships plays a central role in the design and discovery of novel materials. In many cases, developing the relationship between the structure of a new material and its physical and chemical properties requires that measurements be made under exactly the same in-situ conditions of temperature, pressure and atmosphere that match the performance environments of the materials of interest. Examples of research at SNBL leading to a better understanding of materials properties already include catalysis, battery and fuel-cell studies, and solid-state hydrogen storage technology.

Our goal is to develop apparatus for high gas pressure experiments which will enable us to follow gas-solid chemical reactions in-situ using various x-ray methods. The experiments will often be carried out in conjunction with other techniques such as Raman or optical absorption spectroscopy. In addition to the dependence upon gas pressure, we may also wish to vary other experimental parameters such as temperature, humidity, gas-mixture, flow-rate etc. Further information may be obtained by monitoring the gas products using analytical tools such as mass spectrometry. Various X-ray methods including powder and single crystal diffraction, small angle scattering and x-ray absorption spectroscopy may be employed, either separately or in different combinations.

It is evident that an individual cell design will not be able to accommodate all of this wealth of experimental techniques, particularly when we take into account the wide range of gas pressures which we wish to cover (10 bar – 700 bar). In addition, the use of high gas pressures combined possibly with high temperatures and the presence of gas mixtures poses serious challenges for the safe operation of our equipment. Finally, the experiments must be operated remotely, with no manual access to the equipment during data collection. This implies that, as far as possible, we must ensure full automation of the apparatus from the start to the end of the experiment.

We now need to set certain priorities concerning the type of cell (or cells) to use for our in-situ experiments, together with the gas supply set-up (including possibly a gas-mix rig), and the compressor system necessary in order to reach the high pressures. To assist the SNBL team in defining the specification for our reaction cells and associated high pressure equipment, we are holding a two-day workshop at the ESRF on 8 - 9 November 2007. All SNBL users who might be interested in the use of this type of equipment are encouraged to take part in this workshop, so that each group can ensure that their input will be properly taken into account. We are also seeking suggestions concerning possible speakers for this meeting. Note that the

meeting is being organized together with our colleagues from the Dutch/Belgian beamline. Further information will appear in due course on our SNBL web site ([http://www.esrf.eu/exp\\_facilities/BM1A/index.htm](http://www.esrf.eu/exp_facilities/BM1A/index.htm)).

A provisional list of speakers and their topics is given below:

**Paul Barnes** (Brubeck / University College London)

Structure and dynamics of functional materials / cement hydration / hydrothermal crystallization

**Philip L. Llewellyn** (Université de Provence – CNRS, Marseille)

In-situ diffraction experiments, gas/solid reactions in metal-organic framework structures

**Andrew M. Beale** (Dept of Inorganic Chemistry and Catalysis, Utrecht)

In-situ catalysis / combined UV-Vis, Raman and XAFS

**Olga Safonova** (SNBL)

Apparatus for in-situ catalysis experiments

**Wim Bras** (DUBBLE)

Combining SAXS, WAXS and EXAFS for investigating hydrothermal crystallization processes



# Neutronenstreuung für Kristallographen



8.-9. Oktober 2007  
GKSS Forschungszentrum, Geesthacht

Der Arbeitskreis Neutronenstreuung veranstaltet einen Einführungskurs in die Neutronenstreuung mit der speziellen Ausrichtung auf kristallographische Anliegen. Er richtet sich an Studenten, die an Diplom- oder Doktorarbeit arbeiten oder kurz davor stehen, und an alle Wissenschaftler, die einen Einstieg in die Neutronenstreuung suchen.

Die Übersicht der vorgestellten Techniken behandelt Pulver- und Einkristall-Beugungsmethoden zur Untersuchung der Kristall- und magnetischen Struktur, inelastische Streumethoden zur Bestimmung von strukturellen und magnetischen Anregungen, sowie die Analyse der diffusen Streuung aufgrund von nur kurzreichweitiger Ordnung. Der Kurs soll auch in Hinblick auf praktische Aspekte zum Erlangen der Neutronenmeßzeit beraten, also darlegen, wo und wie man Proposal stellen kann. Den Teilnehmern des Kurses wird die Möglichkeit gegeben, eigene Themenstellungen auf Postern vorzustellen und somit intensiv mit den verschiedenen Experten zu diskutieren. Experimentiereinrichtungen an der Geesthacht Neutron Facility (GeNF) können besichtigt werden.

Eine Teilnahmegebühr wird nicht erhoben.

## Montag, 8. Oktober 2007

13:00	Begrüßung	
13:30	Pulvermethoden – Kristallstruktur	Gilles/FRM II
14:30	Pulvermethoden – Magnetismus	Schneidewind/Dresden
15:30	Kaffeepause	
16:00	Einkristalldiffraktion – Kristallstruktur	Meyen/FRM II
17:00	Einkristalldiffraktion – Magnetismus	Braden/Uni Köln
18:00	Postersitzung	

## Dienstag, 9. Oktober 2007

8:30	Spektroskopie – Phononen & Magnonen	Braden/Uni Köln
9:30	Diffuse Streuung	Frey/LMU
10:30	Kaffeepause	
11:00	Materialwissenschaften	Brokmeier/GKSS
12:00	Weiche Materie	Linser/GKSS
13:00	Mittagspause/Abreise	
14:30	Besichtigung GeNF (optional)	

Bitte melden Sie sich online, per e-mail oder per Fax bis zum 21. September 2007 an. Bitte geben Sie auch an, ob Sie ein Poster vorstellen möchten und ob Sie an der Führung durch die GeNF (gültiger Personalausweis oder Reisepaß erforderlich!) teilnehmen möchten:

TU München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II)  
Lichtenbergstraße 1, D-85747 Garching  
Dr. Martin Meyen, e-mail [martin.meyen@frm2.tum.de](mailto:martin.meyen@frm2.tum.de)  
Tel. +49 (0)89 289 147 27, Fax +49 (0)89 289 149 95

## 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	March 15, Nov. 15	<a href="http://user.web.psi.ch">user.web.psi.ch</a>
Protein beam lines (PX)	Feb. 15, June 15, Oct. 15	<a href="http://user.web.psi.ch">user.web.psi.ch</a>
<b>SINQ: Swiss Spallation Neutron Source</b>		
All instruments except imaging	May 15, Nov. 15	<a href="http://user.web.psi.ch">user.web.psi.ch</a>
Imaging	anytime	
<b>SμS: Swiss Muon Source</b>		
All instruments	Dec. 5	<a href="http://user.web.psi.ch">user.web.psi.ch</a>
<b>ESRF: European Synchrotron</b>		
All instruments, long term proposals	Jan. 15	<a href="http://www.esrf.fr">www.esrf.fr</a>
All instruments, short term proposals	March 1, Sept. 1	<a href="http://www.esrf.fr">www.esrf.fr</a>
<b>SNBL: Swiss Norwegian Beam Line</b>		
	March 1, Sept. 1	<a href="http://www.esrf.fr/exp_facilities/BM1A">www.esrf.fr/ exp_facilities/BM1A</a>
<b>ILL: Institut Laue Langevin</b>		
All instruments	Sept. 18, 2007	<a href="http://www.ill.fr">www.ill.fr</a>
<b>FRM-II</b>		
All instruments	26. Jan, 17. Aug.	<a href="http://user.frm2.tum.de">user.frm2.tum.de</a>

## Calendar of Forthcoming Meetings

(please mail missing information on meetings of interest to [Jurg.Schefer@psi.ch](mailto:Jurg.Schefer@psi.ch))

			<b>Abstract Deadline</b>
<b>2007</b>			
June 2 – Sept. 23	Basel CH	Leonhard Euler Jubiläumsprogramm, Naturhistorisches Museum Basel, <a href="http://www.Euler-2007.ch">http://www.Euler-2007.ch</a>	open access
July 8-13	Waterville USA	Gordon Research Conference on "Hydrogen-Metal Systems"	
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>	Expired
August 5-17	Zurich CH	The Zurich Crystallography School <a href="http://www.oci.uzh.ch/diversa/xtal_school">http://www.oci.uzh.ch/diversa/xtal_school</a>	Expired
August 5-11	Turin Italy	41 <sup>st</sup> IUPAC World Chemistry Congress <a href="http://www.IUPAC2007.org">http://www.IUPAC2007.org</a>	Expired
August 5-11	Utah USA	International Summer School on Crystal Growth ISSCG 13 <a href="http://www.crystalgrowth.us/isscg13/index.php">http://www.crystalgrowth.us/isscg13/index.php</a> , Deadline Late News Posters	Expired
August 12-17	Salt Lake City, USA	15 <sup>th</sup> International Conference on Crystal Growth <a href="http://www.crystalgrowth.org/conferences/iccg15/index.php">www.crystalgrowth.org/conferences/iccg15/index.php</a>	Expired
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>	Expired
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> )	Expired
Aug. 22-27	Marrakech Morocco	ECM-24: European Crystallographic Meeting <a href="http://www.ecm24.org">http://www.ecm24.org</a>	Expired
Sept. 3-4	Dublin Ireland	British and Irish Society for Crystal Growth, together with Bernal Symposium, Structural Biology <a href="http://www.bacg.org.uk">http://www.bacg.org.uk</a>	Expired
Sept. 10-13	Nürnberg Germany	Euromat 2007: Advanced Materials and Processes <a href="http://euromat2007.fems.org">http://euromat2007.fems.org</a>	Expired
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>	Aug. 15, 2007
Sept. 12	Villigen PSI CH	Direct methods: Joint SLS-SGK/SSCR session <a href="http://user.web.psi.ch/sls07/prog_direct.html">http://user.web.psi.ch/sls07/prog_direct.html</a>	
Sept. 12-13	Villigen PSI CH	Annual Meeting 2007 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>	Expired
Sept. 21	Villigen PSI CH	Festkolloquium 10 Jahre SINQ	
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>	Expired
Oct. 8-9	Geesthacht Germany	Neutronenstreuung für Kristallographen, DGK contact: <a href="mailto:meven@frm2.tum.de">meven@frm2.tum.de</a>	21. Sept. 2007
Nov. 8-9	Grenoble France	In-situ experiments at SNBL using high gas pressures contact: <a href="mailto:philip.pattison@epfl.ch">philip.pattison@epfl.ch</a>	
Nov. 26-30	Boston USA	MRS 2007 Fall Meeting, Materials Research Society <a href="http://www.mrs.org/s_mrs/sec.asp?CID=4749&amp;DID=164574">http://www.mrs.org/s_mrs/sec.asp?CID=4749&amp;DID=164574</a>	Expired

			<b>Abstract Deadline</b>
<b>2008</b>			
March 3 – 6	Erlangen Germany	16. Jahrestagung der DGK	
March 31-April 4	Villigen PSI CH	Workshop of the INTAS project Spintronics <a href="http://spintronics.web.psi.ch">http://spintronics.web.psi.ch</a>	to be announced
March 9-13	New Orleans USA	The Minerals, Metals and Materials Society (TMS) 2008 <a href="http://www.tms.org/Meetings/Annual-08/AnnMtg08Home.html">http://www.tms.org/Meetings/Annual-08/AnnMtg08Home.html</a>	Expired
April 27– May 3	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
May 29 – June 8	Erice Italy	International School of Crystallography: From Molecules to Medicine, <a href="http://www.crystallerice.org">http://www.crystallerice.org</a>	Nov. 30, 2007
June 9-14	Zurich CH	10th International Conference on Quasicrystals, ICQ10, <a href="http://icq10.ethz.ch">http://icq10.ethz.ch</a>	Jan 15, 2008
August	Osaka Japan	IUCr-2008, 21 <sup>st</sup> General Assembly and Congress of IUCr <a href="http://www.congre.co.jp/iucr2008">http://www.congre.co.jp/iucr2008</a>	to be announced
Sept. 1-11	Warsaw Poland	EPDIC-11 European Powder Diffraction Conference <a href="http://www.epdic-11.eu">http://www.epdic-11.eu</a>	April 15, 2008
Sept. 9-14	Sydney Australia	WATOC-08 World Association of Theoretical and Computation Chemists, <a href="http://www.watoc2008.com/">http://www.watoc2008.com/</a>	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

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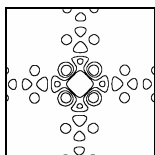
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