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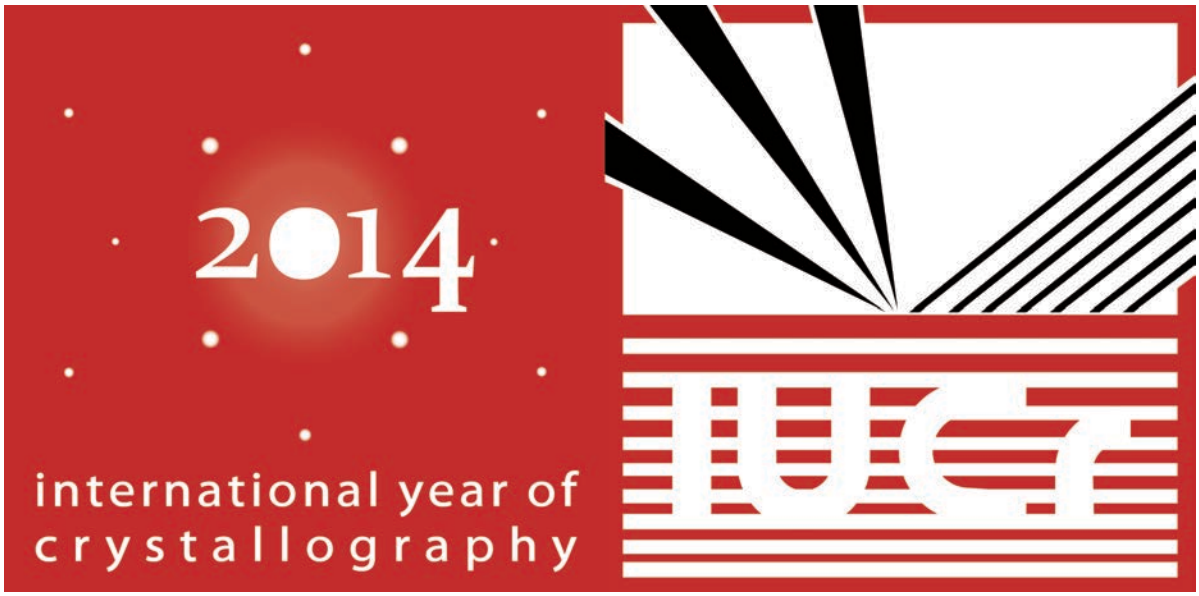

In this issue:

On the Cover:

A Logo of the International Year of Crystallography 2014
Courtesy: http://www.iycr2014.org (UNESCO, IUCr)

The President's Page

2014 – International Year of Crystallography

Every year, the United Nations' Organization is giving special attention to fields of great importance for the international community. Scientific subjects were repeatedly in their focus: 2010 the biological diversity, 2011 chemistry, and next year - 2014 - crystallography. The opening ceremony for this special year will take place on January 20-21, 2014, at the UNESCO headquarters in Paris, the leading organization of the UN for such events. The year of crystallography is also in nice coincidence with the 100th anniversary of the discovery of Bragg's Law in 1912 celebrated last year and many Nobel prizes in this field, awarded for example 1901 to Wilhelm Conrad Roentgen, 1912 to Max Theodor Felix von Laue, 1915 to the two Braggs, just to mention a few of them, opening a completely new science.
Of course, we and our society are very honored by this and will use the opportunity not only to present our field to the public, but also to be present in the science community. We are presently planning a special issue of Chimia, expositions at Swiss Universities, and YOU are encouraged to present our science. We will be glad to support such efforts and can help you by posting your events on our dedicated website.
Especially here in Switzerland, many of us will enjoy chocolate during Christmas time. And also here, learning to control the crystallization process was important, as the fats of cocoa butter crystallize in up to six different forms, and only the best forms should be present to give the best taste. Crystallography is really present everywhere.

Looking forward to a great 2014 !

Jürg Schefer

http://www.iycr2014.org

News for and from members

We welcome the following new members of the SGK/SSCr

Dr. Katarina Stare, University of Geneva
Dr. Anar Singh, PSI Villigen,
Mr. Simone Liuzzi, PSI Villigen
Dr. Julia Dshemuchadse, ETH Zürich

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
- Applicant MUST be a member of our society

If you wish to apply for a travel grant, please send the above-mentioned documents to the president of the SGK/SSCr at any time. You should have been a member for at least one year before applying for a grant.

Travel grants are a good opportunity for young scientists to profit from our society during a period where they have low income. By subsequently becoming a long-term member of our society, you can return this good-will to the next generation.

Details for applications are given at:
http://www.sgk-sscr.ch/TravelGrants.pdf

IUCrJ – a **new fully open-access peer-reviewed journal from the International Union of Crystallography (IUCr)**

The journal will publish high-profile articles on all aspects of the sciences and technologies supported by the IUCr *via* its commissions, including emerging fields where structural results underpin the science reported in the article. Our aim is to make IUCrJ the natural home for high-quality structural science results. Chemists, biologists, physicists and material scientists will be actively encouraged to report their structural studies in IUCrJ.
IUCrJ covers five broad areas:

[1] biology and medicine
[2] chemistry and crystal engineering
[3] materials and computation
[4] neutron and synchrotron science and technology
[5] physics and free electron laser science and technology

The journal has been launched to commemorate the International Year of Crystallography. More details at: http://www.iucrj.org

The SGK congratulates its honorary member, Prof. Jack D. Dunitz on the occasion of his ninetieth birthday.

Jack is a world expert on molecular structure. During his formative years (1944-1957) he has worked in the groups of Dorothy Hodgkin, Linus Pauling and Sir Lawrence Bragg where he made important contributions to coordination chemistry, ligand field theory and organic molecular structure. From 1957 to his retirement in 1990 Jack was Professor of Chemical Crystallography at the Laboratory of Organic Chemistry of the ETH Zurich where he contributed widely to our knowledge about molecular structure: e.g. through conformational analysis of medium rings, with important structural studies on ionophores and the 'Bürgi-Dunitz trajectory' to mention just a few. For more information on Jack's contributions the interested reader is referred to the article "Happy 90th Birthday: Professor Dr. Jack David Dunitz, FRS, the 'Professor's Professor' " and to the references cited there (W. B. Schweizer, R. Gilmour, Helv. Chim. Acta 96 (2013) 539–544).

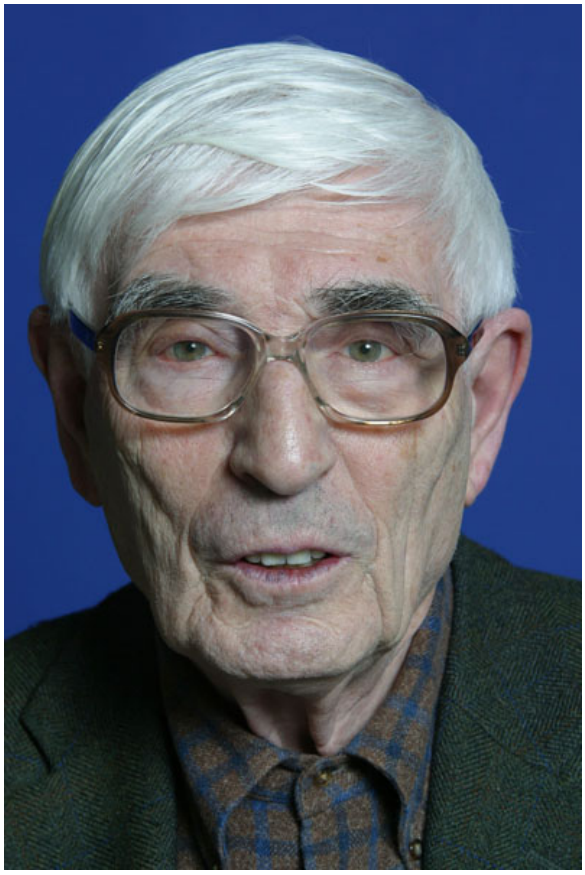

Photo from the web-pages of Academia Europaea: http://www.ae-info.org

To all those who solve their own crystal structures, are uncomfortable with merely pushing buttons on diffractometers and want to understand the basis of what they are doing, we recommend Jack's book 'X-Ray Analysis and the Structure of Organic Molecules' (Verlag Helvetica Chimica Acta, 1995). In spite of its age – it was first published in 1979 - its didactically well-thought-out explanations are far from outdated.

Contributed by Hans-Beat Bürgi

50 Years of Swiss Neutron Diffraction Instrumentation*

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1. Introduction [a b]

Referring to the obituary for Prof. Walter Hälg (1917 – 2011) as Swiss neutron scattering pioneer [1], it may be worthwhile to look at the development of Swiss neutron diffraction instrumentation in the corresponding period of about 50 years.

It depended primarily on the neutron sources, their neutron beam channels, available space for the instruments, on the source operation modes and related decisions.

First the light-water research reactor SAPHIR (Fig. 1) became critical in 1957 with a power of 1 MW. Depending on the experimental needs, the power had been increased in 1970 and 1983 to maximum values of 5 MW and 10 MW, respectively. In December 1993 occured its final shutdown.

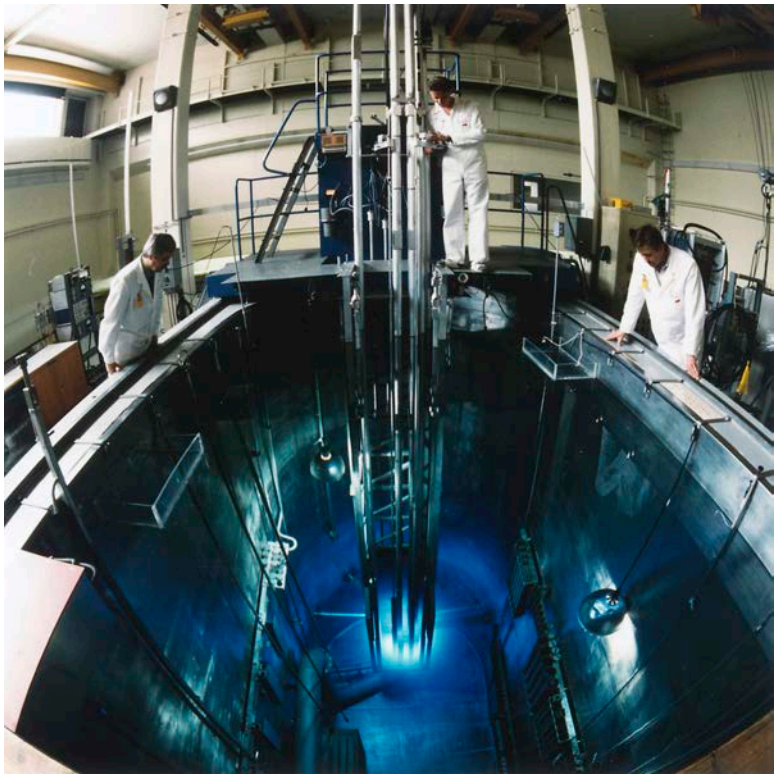


Figure 1: Characteristic Tscherenkow light of reactor SAPHIR (from picture archive PSI).

In the year 1960 the Swiss heavy water reactor DIORIT I became critical. It reached maximum powers of 20 MW (neutron flux 3.5×10^{13} $ncm^{-2}s^{-1}$) and 30 MW in

* This contribution, posthumously dedicated to the Swiss neutron scattering pioneer Prof. Walter Hälg (1917-2011), was originally published in the Swiss Neutron News, Nr. 42 (August, 2013).

the years 1961 and 1966, respectively. In a long shutdown from 1970 to 1972 a new heavy water tank had to be installed.

Then DIORIT II operated until the final shutdown in 1977 with a maximum power of about 24 MW.

From 1988 on Switzerland has officially access to the neutron scattering instrumentation around the high flux reactor of the Institut Laue-Langevin (ILL) in Grenoble. 1994-1998 D1A at ILL could be also partially used in the CRG mode, see section 3.

In the year 1996 the continuous Swiss spallation neutron source SINQ started operation, a project based on ideas of Prof. W. Hälg and realized by a team under W.E. Fischer in cooperation with Prof. A. Furrer et al.

We shall restrict our review mainly on classical powder and single crystal neutron diffraction.

2. Neutron diffractometers at reactors SAPHIR and DIORIT [a b]

During his stay 1952-1953 in Norway Prof. W. Hälg came at the reactor JEEP at Kjeller into contact with neutron scattering. Trained in optical spectroscopy, particle physics as well as in electronics from the University at Basel, he initiated at the swimming pool type reactor SAPHIR the construction of a first two-axes neutron diffractometer (Fig. 2).

Figure 2:
Main mechanical parts of the first neutron diffractometer at reactor SAPHIR, supervised by the mechanics expert M. Koch.

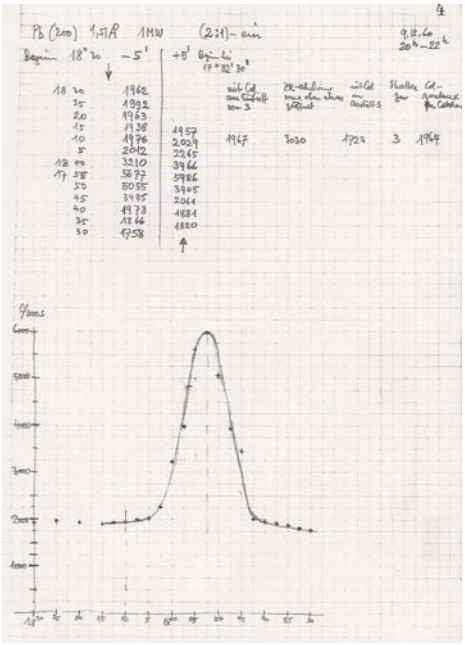


Figure 3:
1.5 Å neutron (200) intensity versus Bragg angle Θ of a Pb crystal, measured by W. Hälg in the θ–2θ mode at reactor SAPHIR at a power of 1 MW.

As at that time electronic controls and computers were only in their beginnings, mechanical 2:1 coupling of the two axes could be used as option, based on the geometrical relations of the central and peripheral angles of a circle.

Such a measurement on a lead crystal, performed manually and noted in 1960 by W. Hälg, is shown in Fig. 3.

Figure 4:
Research team of Prof. Hälg's Delegation AF, approximately 1962: from left W. Hälg, guest G. Ehret from Karlsruhe, P. Fischer, G. Maier, chemist F. Brandt and reactor engineer F. Ferroni.

Dr. Georg Maier, a cousin of the German neutron scattering pioneer Prof. H. Maier-Leibnitz and Peter Fischer as thesis student were the first neutron scattering collaborators of W. Hälg. Fig. 4 shows a corresponding picture at the Swiss Federal Institute for Reactor Research (EIR), Würenlingen.

Together with W. Hälg we first tested neutron monochromators and started optimization of the instrument shielding (Fig. 5) that originally consisted mainly of boron-paraffin blocks and lead.

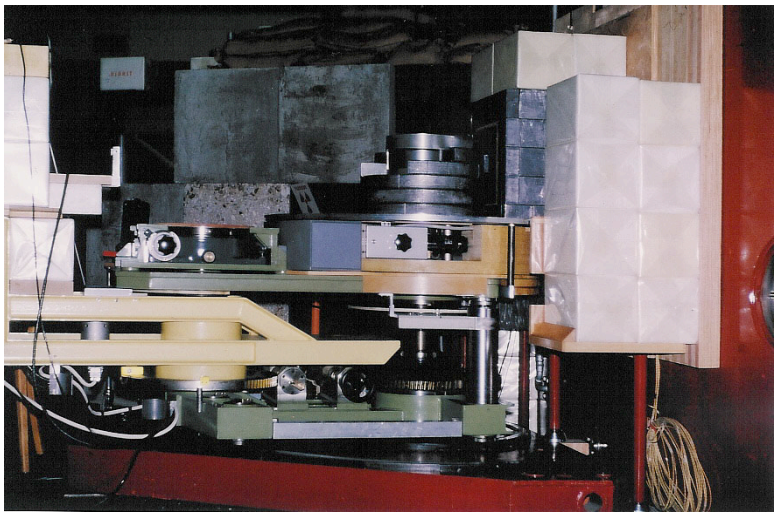


Figure 5:
Installation of the two-axes neutron diffractometer at reactor DIORIT.

As the heavy water reactor DIORIT operated at considerably higher power than reactor SAPHIR, the two-axes neutron diffractometer had been transferred to this reactor. Thus we got practical experience concerning the complementary aspects of thermal neutrons as particles and as waves and also tried to understand theoretically neutron reflectivity from monochromator crystals [2]. On the other hand, G. Maier developed first programs to calculate neutron structure factors and for data evaluation at a Zuse computer of EIR.

Other necessary devices such as plugs, Soller collimators or crystal holders had been realized in collaboration with the workshop group under the supervision of W. Hälg and the workshop chief E. Härdi from EIR.

With respect to long measuring times automation of data collection had been necessary. Due to his electronics experience W. Hälg created soon a corresponding working group for this important project. A first result for the powder neutron diffractometer at reactor DIORIT is shown in Fig. 6.

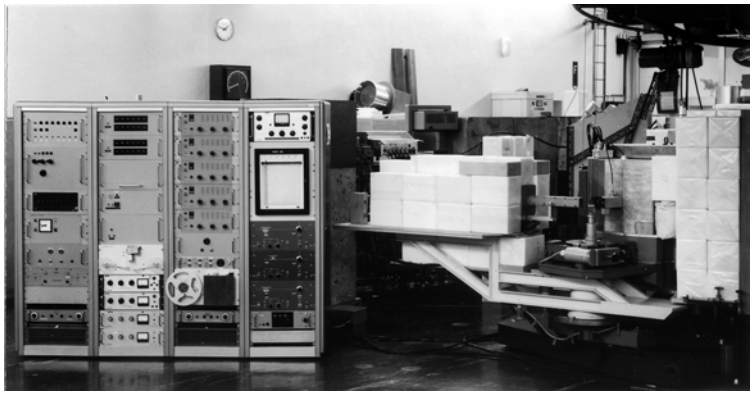


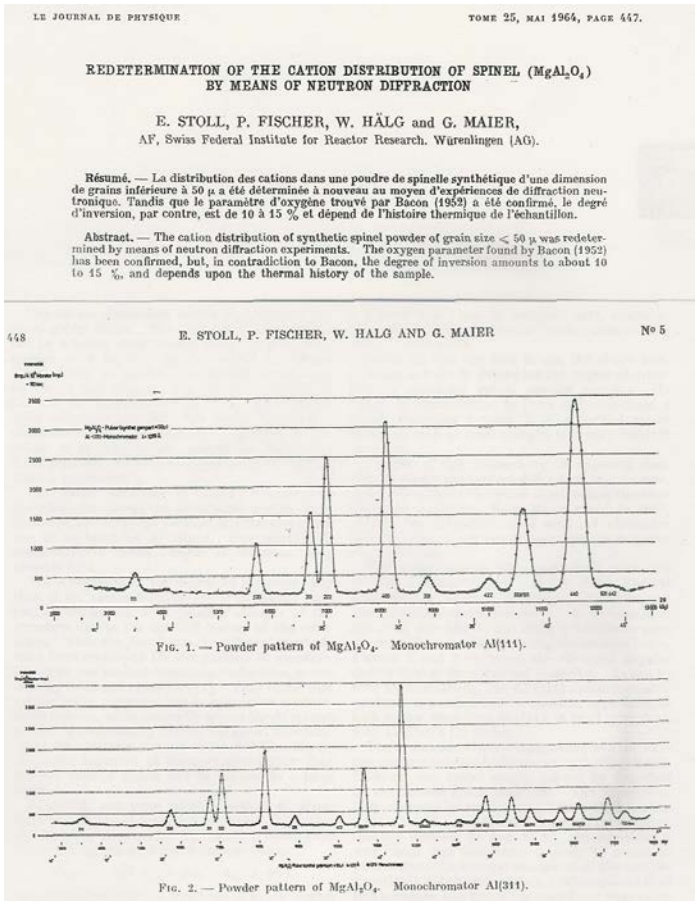
Figure 6:
Powder neutron diffractometer with automatic data collection by means of paper tape input and output at DIORIT I.

Figure 7:
Optimized detector shielding at DIORIT I with optional counter tilting for single crystals.

Concerning the detector shielding W. Hälg proposed to test the possibility to position the detector accurately and to let the heavy shielding follow the detector movement. As for focusing the detector has to turn towards the monochromator shielding, later a more compact detector shielding such as shown in Fig. 7, combined with good monochromator shielding, resulted in considerably improved experimental conditions. Such efforts yielded 1964 a first neutron powder diffraction publication, see Fig. 8.

Occasionally also Prof. Paul Scherrer (Fig. 9) passed by at the neutron diffractometer and checked wether the powder sample was properly rotating at room temperature according to the Debye-Scherrer method.

Fig. 10 illustrates the enlarged team of W. Hälg 1970 contributing to neutron scattering. Willi Bührer developed also with Swiss mechanical precision single and double focusing monochromator systems, in particular when suitable pyrolithic graphite became available.



LE JOURNAL DE PHYSIQUE — TOME 25, MAI 1964, PAGE 447.

REDETERMINATION OF THE CATION DISTRIBUTION OF SPINEL ($MgAl_2O_4$) BY MEANS OF NEUTRON DIFFRACTION

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AF, Swiss Federal Institute for Reactor Research, Würenlingen (AG).

Résumé. — La distribution des cations dans une poudre de spinelle synthétique d'une dimension de grains inférieure à 50 μ a été déterminée à nouveau au moyen d'expériences de diffraction neutronique. Tandis que le paramètre d'oxygène trouvé par Bacon (1952) a été confirmé, le degré d'inversion, par contre, est de 10 à 15 % et dépend de l'histoire thermique de l'échantillon.

Abstract. — The cation distribution of synthetic spinel powder of grain size < 50 μ was redetermined by means of neutron diffraction experiments. The oxygen parameter found by Bacon (1952) has been confirmed, but, in contradiction to Bacon, the degree of inversion amounts to about 10 to 15 %, and depends upon the thermal history of the sample.

448 E. STOLL, P. FISCHER, W. HALG AND G. MAIER N° 5

FIG. 1. — Powder pattern of $MgAl_2O_4$. Monochromator Al(111).

FIG. 2. — Powder pattern of $MgAl_2O_4$. Monochromator Al(311).

Figure 8:
Improved neutron powder diffraction resolution due to increase of the scattering angle of the monochromator.

Figure 9:
Monument plate for Walter Boveri and Paul Scherrer stating the successful start of the first Swiss reactor DIORIT.

Figure 10:
Group photo 1970 of the collaborators of W. Hälg (left) and EIR contributing to neutron scattering. Note the Swiss pioneers W. Bührer and A. Furrer for inelastic neutron scattering in the front row from right.

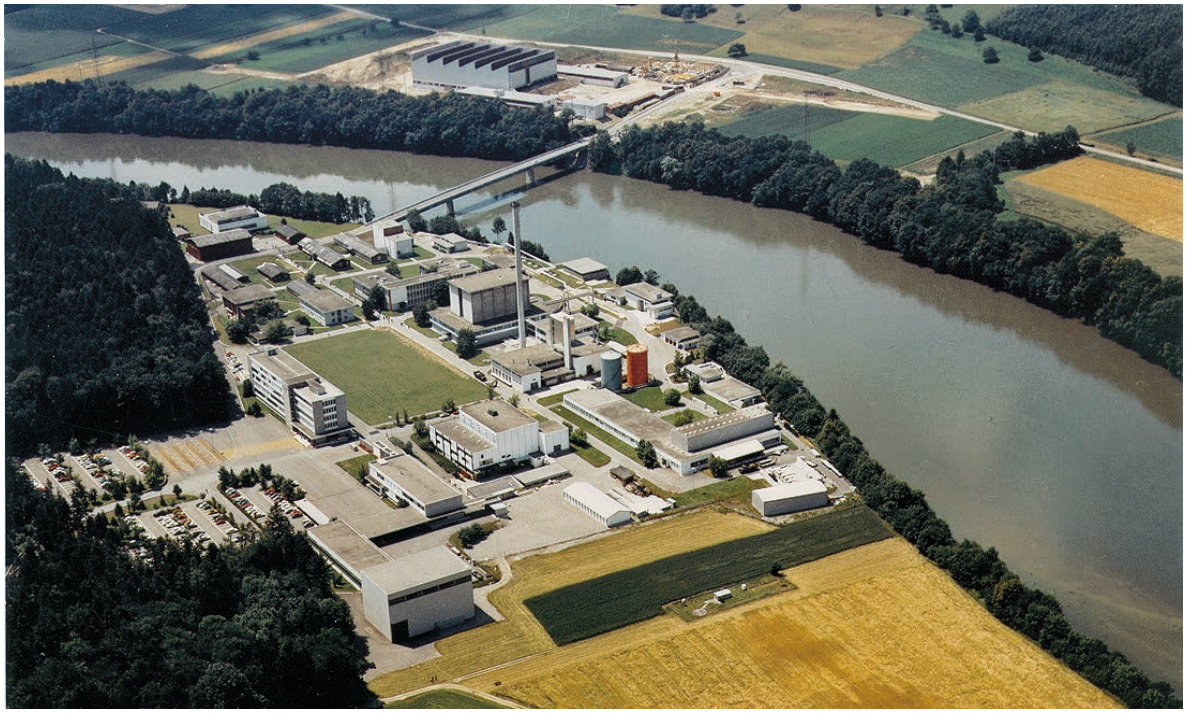

Figure 11: EIR and SIN 1971.

Fig. 11 is an aerial view of both institutes EIR and SIN (Swiss Institute for Nuclear Research) in 1971. The large building left of the high chimney is the one of reactor DIORIT. And left, almost hidden by trees, one can see the building of reactor SAPHIR.

Because of the upgrading period 1970-1972 from reactor DIORIT I to II, reactor SAPHIR's power had been increased in the year 1970 to 5 MW. And a part of the neutron instrumentation including two-axis diffractometers had been installed there. Because of the space limitations with at maximum three beam tubes this had been a difficult time for the Swiss neutron community.

Fig. 12 shows the final neutron scattering instrumentation at reactor DIORIT II in the years 1972-1977, characterized by movement of heavy loads on air cushions. At the right side of the central triple-axes neutron spectrometer one may recognize the two-axis neutron diffractometer, used for single crystal studies of magnetic phase diagrams in external magnetic fields up to 60 kG. With a vertically focusing pyrolithic graphite monochromator since 1974 remarkable intensity gains had been obtained. On the left side in the front K. Tichy had installed together with Prof. J. Benes a first four-circle neutron diffractometer for single crystals, see e.g. ref. [3]. The data collection had been done by means of a central CDC 8090 computer. Both at DIORIT and at SAPHIR helium gas recovery systems had reduced the costs for liquid helium essentially.

Figure 12:
Neutron scattering instrumentation at reactor DIORIT II, 1972-1977.

Due to the final shutdown of reactor DIORIT (to reduce costs) neutron instrumentation had been again transferred to reactor SAPHIR in an increased experimental hall, see Fig. 13. To improve the background conditions, also BeO elements had been installed in the reactor. In 1983 SAPHIR reached the maximum power of 10 MW. Thus the neutron intensity became approximately comparable to the one of DIORIT II with 24 MW.

Since 1975 to his retirement in 1984 W. Hälg had been the head of the neutron scattering group within his Institute for Reactor Technics (IRT) at ETHZ. He always made the neutron instrumentation available to a broad national and international user community and introduced a fair user system to distribute the beam time.

In addition he organized national discussion meetings in 1973, together with Prof. H. Gränicher as director of EIR. In 1978 he also presented in another discussion meeting with B. Sigg first ideas for a SINQ spallation neutron source.

At SAPHIR with H. Heer as coordinator each instrument had been controlled by means of a PDP 11 and later LSI 11 computer, thus permitting online data evaluation.

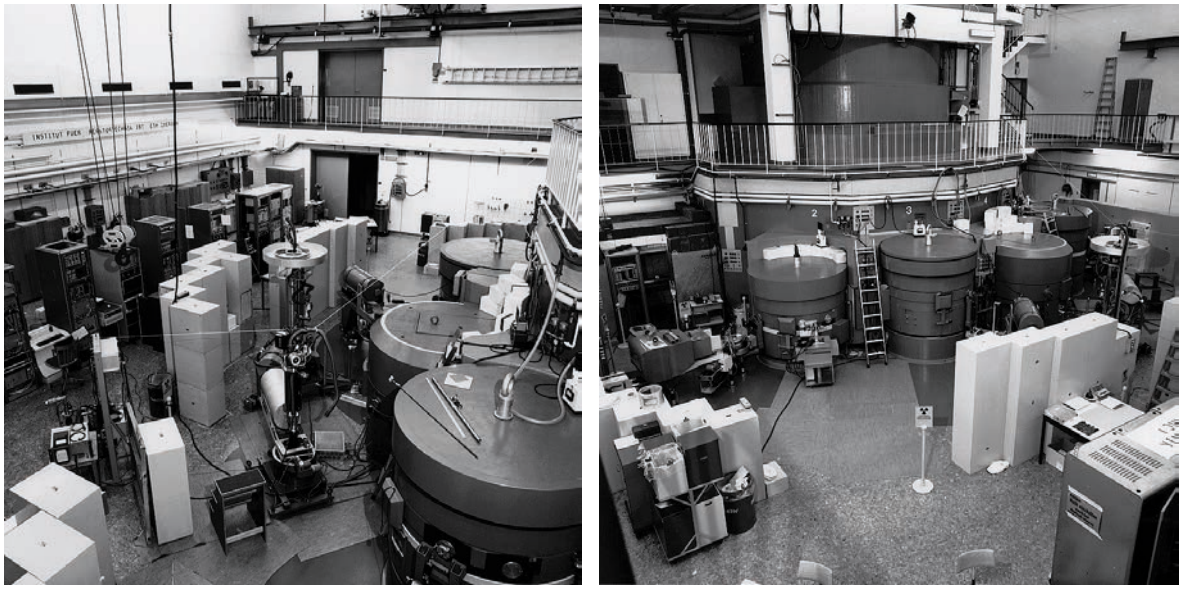

Figure 13:
Neutron instrumentation at reactor SAPHIR 1983 with two-axis neutron diffractometers visible in the center of the pictures a) and b).

In order to increase with medium neutron flux substantially the performance of the powder diffractometer, W. Hälg et al. started as successful teamwork the realization of the double-axis multicounter neutron powder diffractometer DMC [4,5]. It is illustrated in Fig. 14. This project had been financially supported by several Swiss institutes. And after now almost 30 years of operation this instrument is still well demanded at SINQ, using cold neutrons, see section 4.

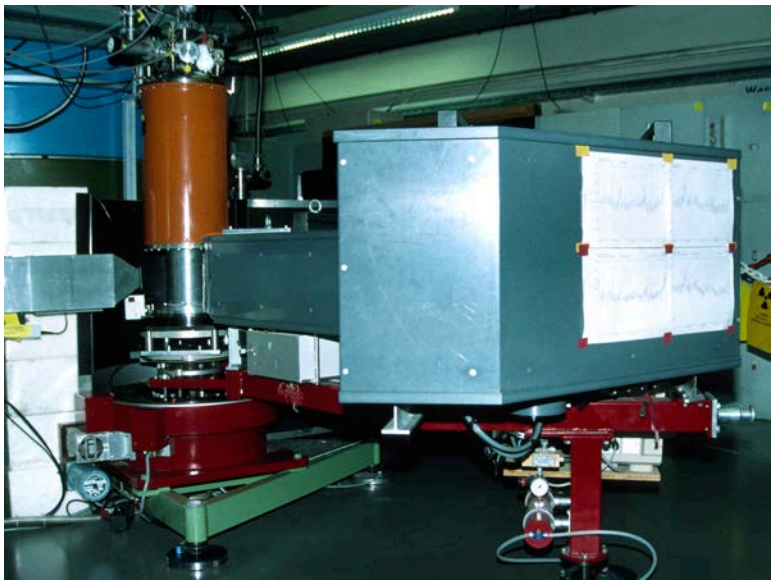

Figure 14:
Final state 1993 of DMC with 400 BF_3 detectors covering a scattering angle range of 79.8 degrees, radial collimator, optional 10' mylar type primary collimator, vertically focussing pyrolithic graphite and Ge monochromators at the 10 MW reactor SAPHIR.

Also Prof. A. Furrer - succeeding Prof. W. Hälg in 1984 - actively promoted instrumental development as head of the Laboratory for Neutron Scattering, ETH Zurich. In particular he looked for important auxiliary equipment, such as a dilution refrigerator reaching 7 mK (Fig. 15). Fig. 16 illustrates the neutron scattering group at that time.

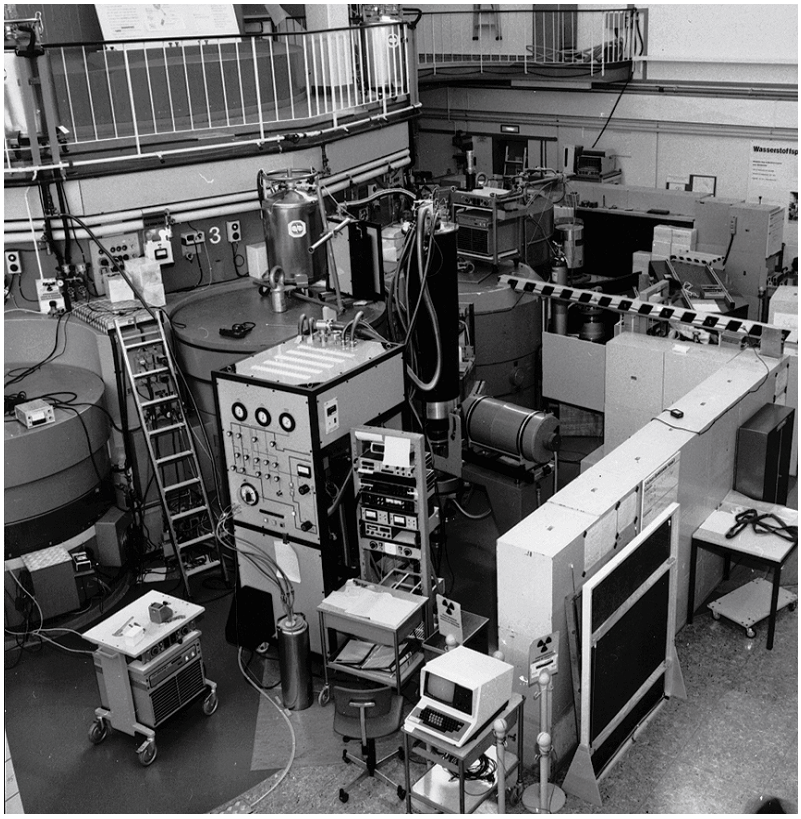

Figure 15:
7mK refrigerator used 1988 on the two-axis neutron diffractometer P2AX@SAPHIR.

Figure 16:
Neutron scattering group 1988.

Finally in Fig. 17 the new 4-circle neutron diffractometer of J. Schefer with closed-cycle cooling machine and single detector is shown.

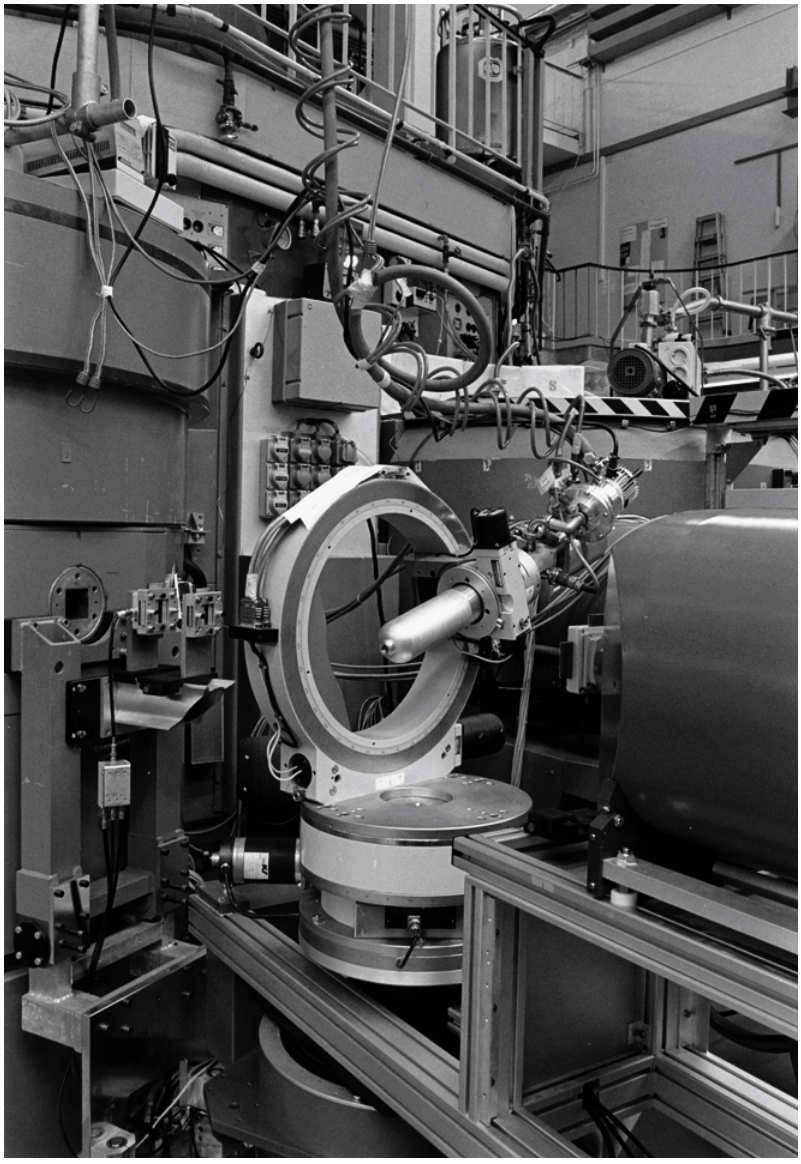

Figure 17:
New four-circle neutron diffractometer 4C 1992 at reactor SAPHIR.

3. D1A as 'half Swiss' CRG instrument [a]

From 1994 to 1998 Swiss users had between the shutdown of reactor SAPHIR and the startup of SINQ the opportunity to use up to 25 % of the D1A beam time at ILL in the CRG ('collaborative research group') mode for their research and for training of thesis students. In this period this first high-resolution powder neutron diffractometer of ILL [6] had 25 mylar type Soller collimators and ^{3}He detectors. And F. Fauth operated the instrument as local contact very well.

4. Cold neutron powder diffractometer DMC at SINQ [ch]

For the start of the Swiss Spallation Neutron Source SINQ in 1996 DMC was moved and adapted to the SINQ guide hall and has been operated since then as a cold neutron diffractometer. Located at an m = 2 supermirror neutron guide (Fig. 18), it is used without primary collimation and with optional secondary collimation providing maximum intensity. With the cold neutron spectrum (2.3 Å < λ < 5 Å), the focusing pyrolytic graphite monochromator and the low background due to optimized shielding, DMC is designed for efficient diffraction studies in the fields of crystallography, solid state physics and material science, in particular for the determination of weak intensities. Although its momentum transfer range Q is limited, its resolution exceeds the one of HRPT at smaller Q values. Special features are the linear position sensitive detector (BF_3, angular coverage 79.8°), the oscillating radial collimator system to suppress scattering from the sample environment and a large diversity of available sample environment devices, cf. http://www.psi.ch/sinq/dmc/.

A high-resolution option is provided by the optional vertically focusing Ge monochromator. Designed complementary to the thermal instrument HRPT, typical experiments on DMC are the determination of magnetic structures, the efficient measurement of magnetic or crystallographic phase transitions, and the analysis of large unit cell structures.

Figure 18:
High-intensity multidetector powder diffractometer DMC for cold neutrons at SINQ.

Planned upgrades of the instrument include the replacement of the aging detector electronics and the installation of a nonmagnetic sample table to further broaden the range of applications for DMC, in particular for investigations in external magnetic fields.

Standard for the control of SINQ instruments is the SICS client server system [7]. With it the instrument is locally supervised from the instrument computer, but measurements may be also controlled remotely. And for online data evaluation either PC-s with Linux software or Mac-s are available.

5. High-resolution powder diffractometer HRPT for thermal neutrons at SINQ [a e f]

HRPT [8] is situated at the target station of SINQ (Figs. 19 and 20), using thermal neutrons from a water scatterer in a tangential beamtube. Complementary to DMC it is designed as flexible instrument for both high-intensity and high-resolution investigations (see measured high-resolution functions shown in Fig. 21). In view of the medium neutron flux of SINQ and uncertainties at the beginning of SINQ operation concerning possible shielding problems due to the high energy spallation neutrons, this powder neutron diffractometer is based on a vertically focusing wafer-type Ge(hkk) monochromator, a radial collimator of mylar-GdO type and a large multidetector with 1600 wires and angular separation of 0.1 degrees between adjacent wires. The fixed monochromator takeoff-angles of 90 and 120 degrees ensure short monochromator-sample distances.

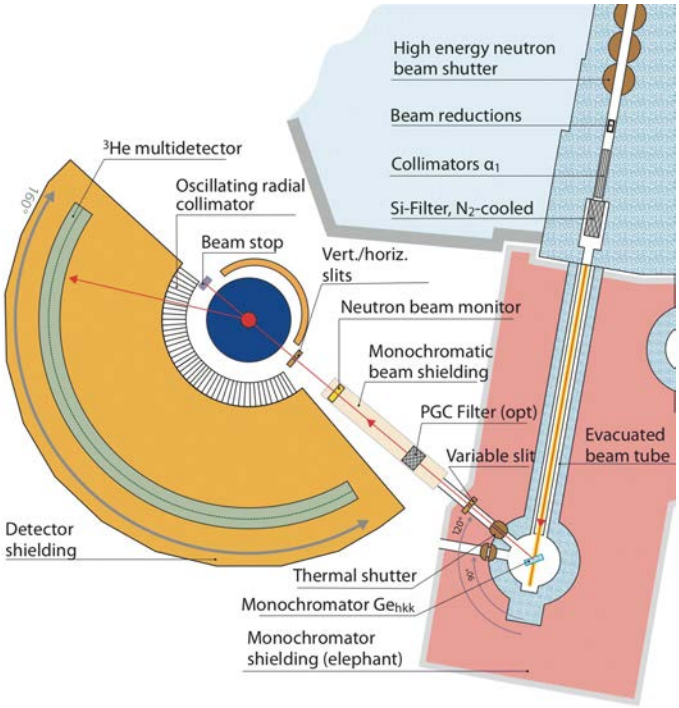

Figure 19: Layout of HRPT.

HRPT is designed as flexible instrument for efficient neutron powder diffraction studies in novel materials concerning chemical structures and magnetic ordering for large ranges of parameters such as temperature and pressure - also for small sample sizes. By means of a set of primary collimators, a secondary slit system and by appropriate choice of the sample diameter, resolution and intensity can be adapted to the needs, see http://www.psi.ch/sinq/hrpt/. The multidetector can be accurately positioned on air cushions.

The data transfer from the fast frontend field-programmable gate array FPGA, designed and programmed at PSI, to the user interface and histogram memory is made via a central data exchange system and optical cables.

The high number of channels and high electrical voltage (~7kV) provoke continuous occurrence of sporadic discharges that can lead to the appearance of false counts ('spikes'). Several hardware and software filters are implemented. A blocking trigger installed in FPGA filters these 'discharges' by making use of their synchronous appearance in several non-neighbouring wires. The critical high voltage sockets are now continuously flushed with nitrogen gas. The detector is very well shielded also from the fast SINQ neutrons. As a result of all the above efforts the background conditions are very good, allowing measurements of rather small samples.

Figure 20:
High-resolution powder diffractometer HRPT@SINQ for thermal neutrons with multidetector and electronics.

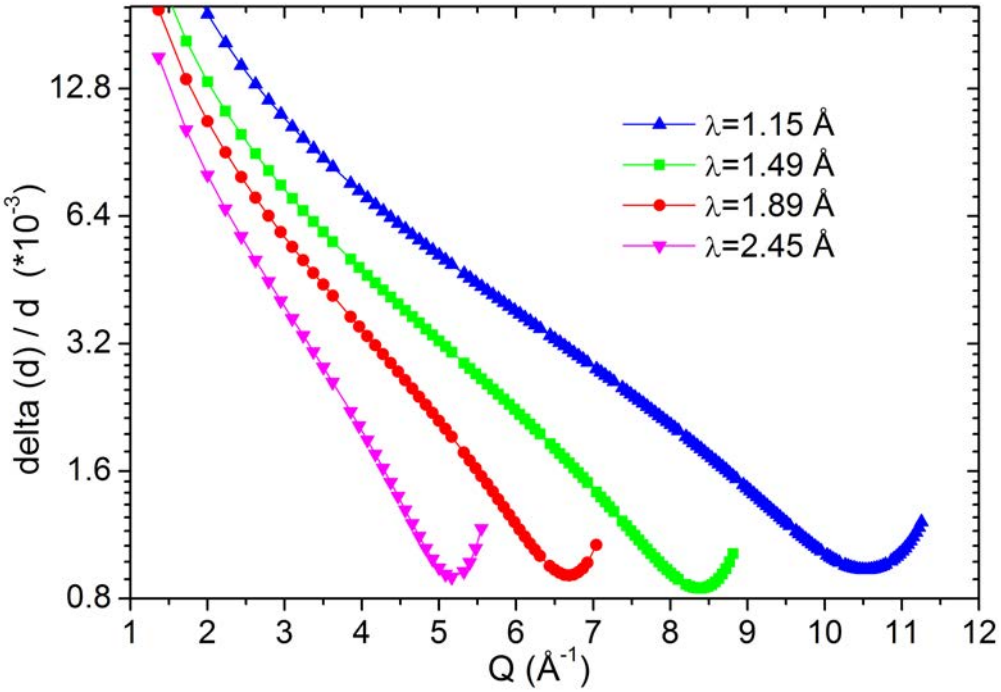

Figure 21:
Measured high-resolution functions δd/d (α_1=6', α_2=12', radial collimator 2, sample diameter 6 mm) of HRPT for $2\theta_M$=120° as functions of available neutron wavelengths and momentum transfer Q. d is the lattice spacing.

In the last decade important new auxiliary devices/possibilities such as a platform for convenient sample handling, cooling liquids etc., were added. It is illustrated in Figs. 22a) and b).

One may now choose between two oscillating radial collimators (FWHM = 7mm and 14mm) to suppress Bragg peaks from the sample environment such as from cryostats, furnaces, magnets or high pressure cells (< 14 kbar) and (< 100 kbar).

For the fine sample positioning in the scattering plane, there is a motorized xy-table controlled by computer. The accuracy of the sample positioning with respect to the detector center of about 0.5 mm is achieved by a special measurement of the standard sample and quick automatic refinement by a script. The positioning is very important for accurate determination of atomic displacement parameters ADPs.

Figure 22:
Platform on top of HRPT.

HRPT is also equipped with computer controlled sample changers for either eight samples at room temperature or for four samples for the temperature range of (1.5 - 315) K.

A very small leak in the detector results in a slow continuous decrease in the gas mixture pressure and worsening of the detector PHS spectrum. Therefore a special cleaning/ pressurizing system has been designed at PSI and manufactured by the MESSER Schweiz company. The system allows for effective cleaning of the gas mixture and removes the impurites such as O_2, N_2, H_2O, etc. by a circulation of the gas mixture through appropriate filters without a need for pumping out the detector.

The instrument is controlled via the SICS and SEA softwares developed by LDM/PSI for a UNIX workstation, permitting fully automatic computer controlled measurements, data reduction and rapid online refinements.

The HRPT instrument is not only used for academic science in the frame of the SINQ user policy program, but also a limited amount of HRPT beam time is available to interested industrial companies. Certain companies cannot disclose the details of their research for confidentiality reasons, and in this case HRPT beam time can be purchased according to the PSI rules.

A further improvement of HRPT would be a second monochromator such as Ge, optimized for 2.45 Å.

6. Single-crystal neutron diffractometer TriCS at SINQ [b d g]

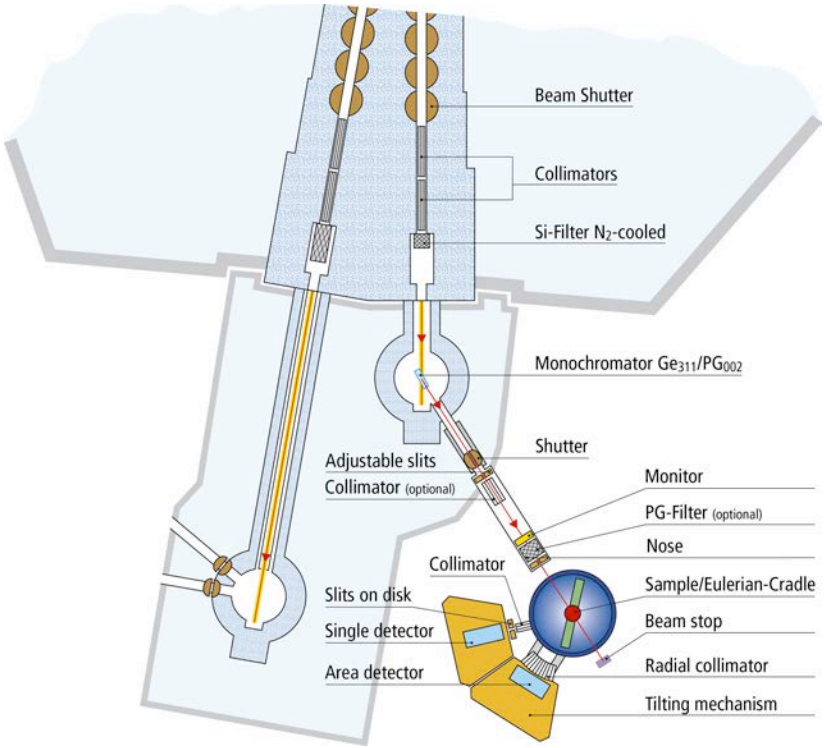

Figure 23:
Present layout of the single crystal neutron diffractometer TriCS@SINQ.

The single crystal neutron diffractometer TriCS [9] (Figs. 23,24), see also http://www.psi.ch/sinq/trics/ , has been designed for solving structural problems in chemistry (λ=1.18 Å, Ge(311), maximum $\sin(\theta/\lambda)$=0.7 $Å^{-1}$) as well as in magnetism (λ=2.31Å, PG(002)). It has been successfully operated for 15 years on a thermal beam tube at SINQ.

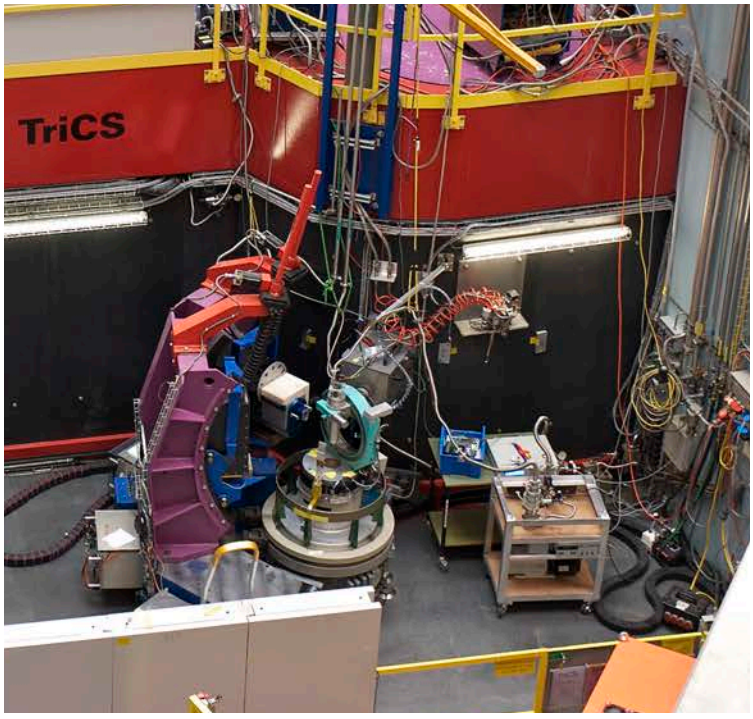

Figure 24:
Single-crystal four-circle neutron diffractometer TriCS for thermal neutrons at the SINQ target station.

Unique features are the tilting option allowing bulky equipment such as magnets and the possibility to switch within minutes from a single tube ^{3}He detector to a two-dimensional area detector (160mm by 160mm, radial collimator, time-delay readout).

Future developments in progress will not only increase the flux by an improved primary optics and the new vertically focusing PG monochromator (SwissNeutronics), to be installed in 2013, but also dramatically reduce the background as a result of improved shielding, based on state-of-the-art absorption calculations. A key issue in this new instrument ZEBRA (Fig. 25) - presently in the predesign phase - will be the optional analyser in front of the single detector. ZEBRA will also yield much faster data collection by removing air cushions. The complete unmagnetic construction will allow higher magnetic fields up to 12 Tesla. ZEBRA also will be suitable for smaller crystal volumes as required by investigations of novel materials, for example in the field of multiferroics.

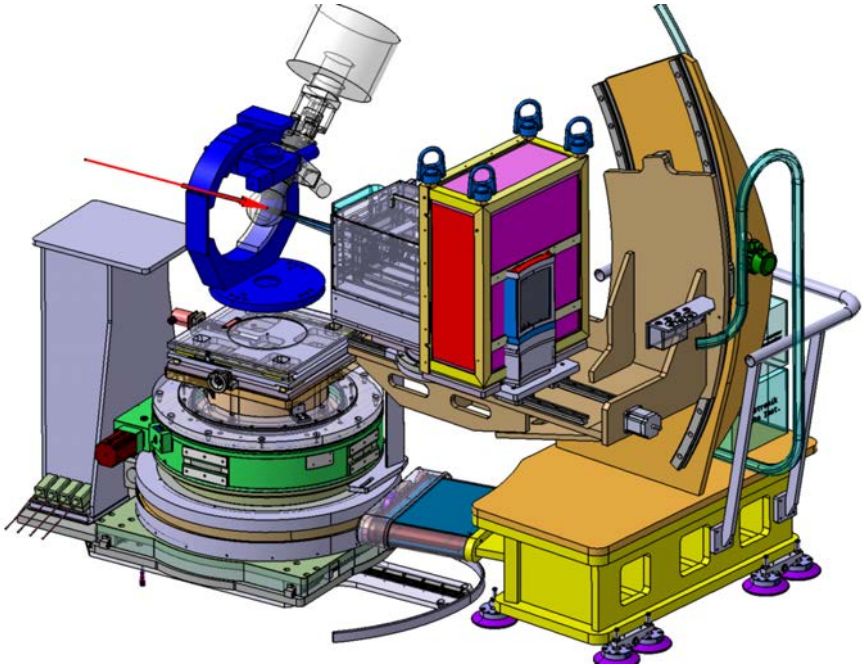

Figure 25:
ZEBRA, the new single crystal neutron diffractometer at SINQ (design phase), replacing TriCS.

New software developments will assist less experienced users to benefit from all the options available. We continue here improvements such as possibilities to create 3D-cuts in q-space for TriCS data collected with the 2D-detector.

In summary, the new ZEBRA will focus on investigation of magnetic structures with the possibility to use externel magnetic fields up to 12 Tesla, but also will improve crystallographic investigations on dedicated systems as presently covered by TriCS, with lower data collection times. Zebra will be funded in part by the Swiss National Science Foundation (Requip).

7. HEIMDAL hybrid neutron spectrometer project at the European Spallation Neutron Source ESS: Probing multiple length scales in one instrument [g i k b j]

Ongoing improvements in material performances are reached for example by the incorporation of advanced ceramics and polymers into heterogeneous systems. Their performances usually depend on the interplay between properties defined by the atomic, nano/mesoscopic and microscopic structure. Traditionally such structural information is collected in separated experiments such as wide angle diffraction (probing the atomic scale, 0.3 $Å^{-1} \leq Q \leq 50\ Å^{-1}$), small angle scattering (nano/meso scale, $0.002\ Å^{-1} \leq Q \leq 0.1\ Å^{-1}$) and direct space imaging techniques (sub-millimeter to millimeter scale).

The hybrid instrument HEIMDAHL [10] (Fig. 26), is proposed by a collaboration of the universities of Aarhus and Copenhagen as well as the LNS, to be built at the European Spallation Neutron Source ESS (Lund, Sweden).

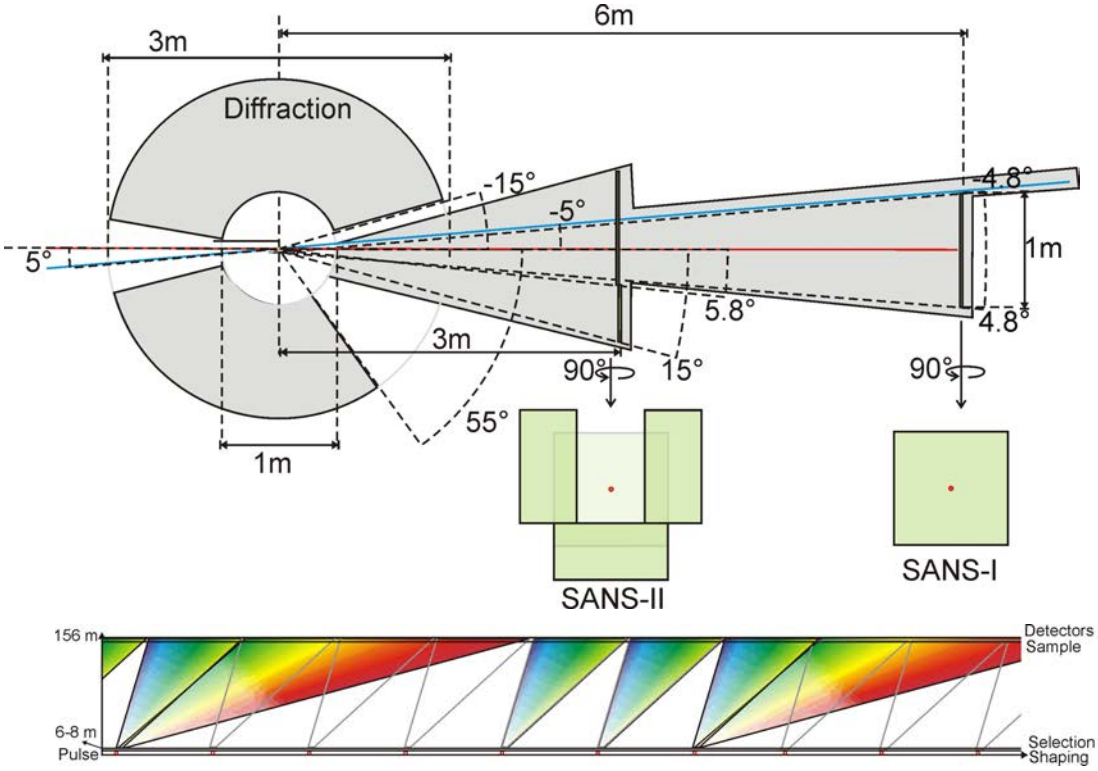

Figure 26:
A schematic illustration of the combined powder diffraction and SANS setup. Below is the pulse train, where three diffraction pulses are skipped to allow a longer SANS pulse. Other operations modes are possible depending on the used choppers sequence. The short wavelength pulse and the long wavelength pass are transported through different guides due to different needs for the neutron optics.

The instrument is designed to obtain a coherent multilength scale picture of these materials. The idea is to merge neutron powder diffraction (probed length z ~ 0.01-5 nm), small angle neutron scattering (z~1-500 nm) and neutron imaging (z~0.01-100 mm), giving a huge advantage, especially for in situ measurements. To fit these needs, the instrument will have two guide systems looking on different parts of the source (thermal and cold) through a single beam port.

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Presenting on Confined Fluids at the X-ray Science 2013 Gordon Conference

Contributed by Simone Liuzzi,
PhD Student at the Confined fluids group, Paul Scherrer Institut

The Gordon Conference X-ray Science 2013 was held at Stonehill College in Easton, Massachusetts from August, from 4 to 9 August. It was preceded by a two-days Seminar on the same topic, addressed mostly to PhD students and postdocs.
These were seven fruitful days, attended by many of the most important players in the field, mostly from synchrotron facilities and universities in the USA and Europe. Since Gordon Conferences follow a policy of presenting "off the record" unpublished results, the details of the topics presented by other attendees should not be disclosed here, but it is worth noting the community's growing excitement for the perspective of diffraction limited storage rings.
I would like to acknowledge the Seminar + Conference formula. Not only does it fulfill its declared goal of allowing younger scientists to present their results in front of an international audience in the form of an oral presentation, it also offers the opportunity for discussions between peers in a more informal setting. This has the positive side effect of increasing the confidence of younger attendees right before the main event takes place. Only a few Swiss scientists were present at the conference. Nonetheless the names of several Swiss professors and scientists appeared in talks or posters of collaborators, and SLS was often referred to as a stable and reliable light source.
Supported by a travel grant from the Swiss Society for Crystallography, I could present in a Seminar talk and as a poster the results of a collaboration between several institutions of the ETH domain: PSI-SLS (Shirish Chodankar, S.L. J. Friso van der Veen, Manuel Guizar-Sicairos and Ana Diaz), the department of materials at ETH-Zürich (Rosa Espinosa-Marzal) and EMPA St. Gallen (Manfred Heuberger).
The collaboration studies the arrangement of atoms and molecules of fluids confined in a nanometer sized gap, a situation in which the combination of interfacial effects and size often confers to the system properties much different from those observed in bulk fluids [1,2]. In particular, understanding the structure of electrolytes confined between two aluminium-phyllosilicate walls could be enlightening in a number of fields, ranging from biology to nuclear waste management, as well as clarify some fundamental issues regarding alkali hydration energies and their influence on the surrounding hydrogen bond network.
We have adapted the extended surface force apparatus (eSFA) developed at ETHZ to be used as a confinement device for X-ray reflectivity (XRR) experiments conducted at the cSAXS (XSA12) beamline of the Swiss Light Source at PSI.
The eSFA uses optical interferometry to measure the distance D between two mica surfaces glued to two cylindrically shaped supports at their point of closest approach. One of the holders is connected to a spring of known elastic constant and they can be moved closer or separated by an actuator. The difference between the imparted movement M and the actual variation in D yields the net force F (attractive or repulsive) acting between the surfaces [2].
In a traditional SFA, the cylindrically shaped supports are made of silica and fully back the mica membrane. For the purpose of the X-ray experiments, such holders have been substituted with metal holders having a slit so as to allow the beam to illuminate the contact area and be scattered toward the detector without obstacles [3].

Two cylindrically shaped and locally unsupported mica membranes form, when pressed together, a flat circular contact area having a typical diameter of ca 500 µm. The pair of membranes serves as confinement device for the liquid trapped between them. X-ray radiation will be scattered by the whole mica-liquid-mica system (including water adsorbed on the outer surfaces), and the mathematical expression for the structure factor intensity $|F(q)|^2$ includes all the contributions and their interference [3].

If the scattered intensity is measured at an angle equal to the incidence angle, the momentum transfer is normal to the surface, and the technique is therefore sensitive to out-of-plane variations in the electron density.

We have performed X-Ray Reflectivity (XRR) experiments from the contact area as a function of the momentum transfer q ranging from 0 to 60 nm^{-1}. Model dependent fits to the measured reflectivity allowed us to determine the minimum gap distance and the electron density profile along the confinement direction [3,4].

In a first set of experiments, the natural layer of K^+ ions present on cleaved mica surfaces was substituted with monovalent Rb^+ or divalent Sr^{2+} ions. The ion-exchanged membranes were brought into contact in a nitrogen environment with controlled relative humidity (RH). XRR measurements were then made at 0 and 60 % RH.

In the second set of experiments, droplets of RbCl, CsCl and $BaCl_2$ solutions at different concentrations were confined. In order to achieve confinement, we chose sufficiently high concentrations with Debye length λ_D<1 nm so as to screen out double layer repulsion between the membranes and allow attraction between them.

We have quantitatively determined the minimum gap distance between the mica surfaces under a small applied pressure for different surface ions and confined electrolytes. In all cases we have observed layered electron density profiles within the gap as we did for natural mica and water in [4], with the layering generally being stronger than at a comparable distance from a single surface. A comparison between confined chloride solutions with different monovalent and divalent cations (Cs^+, Rb^+ and Ba^{2+}) reveals cation specific effects which can be related to concentration, ion size and hydration behavior. A particularly strong layering is observed for concentrated divalent salt solutions. We attribute the latter to ion-ion correlations effects. In monovalent electrolytes, the position and width of the layers are consistent with literature values for single salt/mica interfaces [6].

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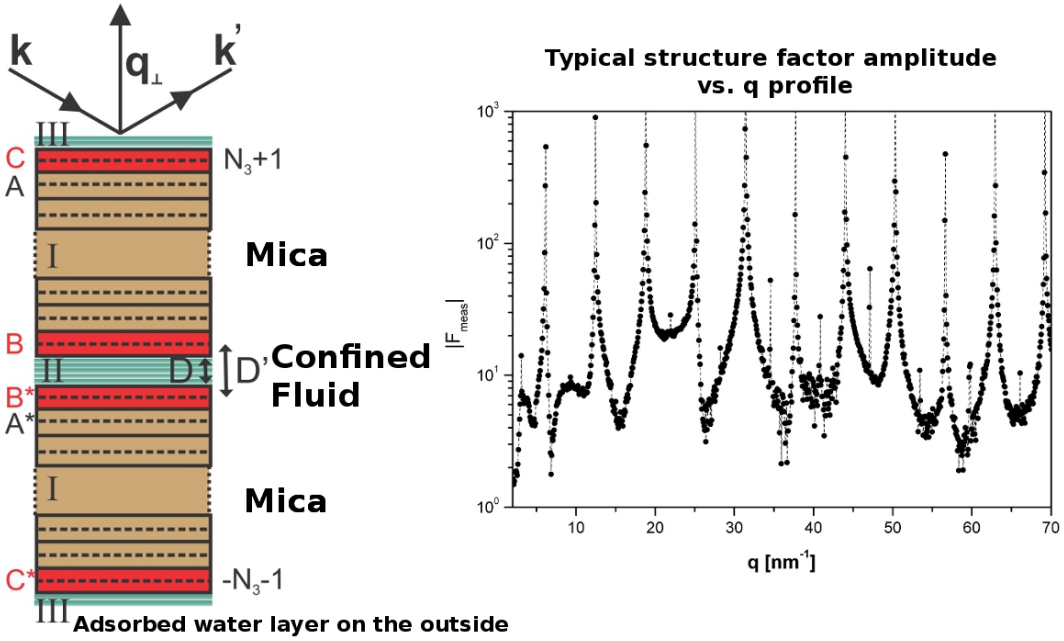
Fig 1. Confinement geometry (left) and a typical X-ray reflectivity structure factor as a function of momentum transfer *q* (right).



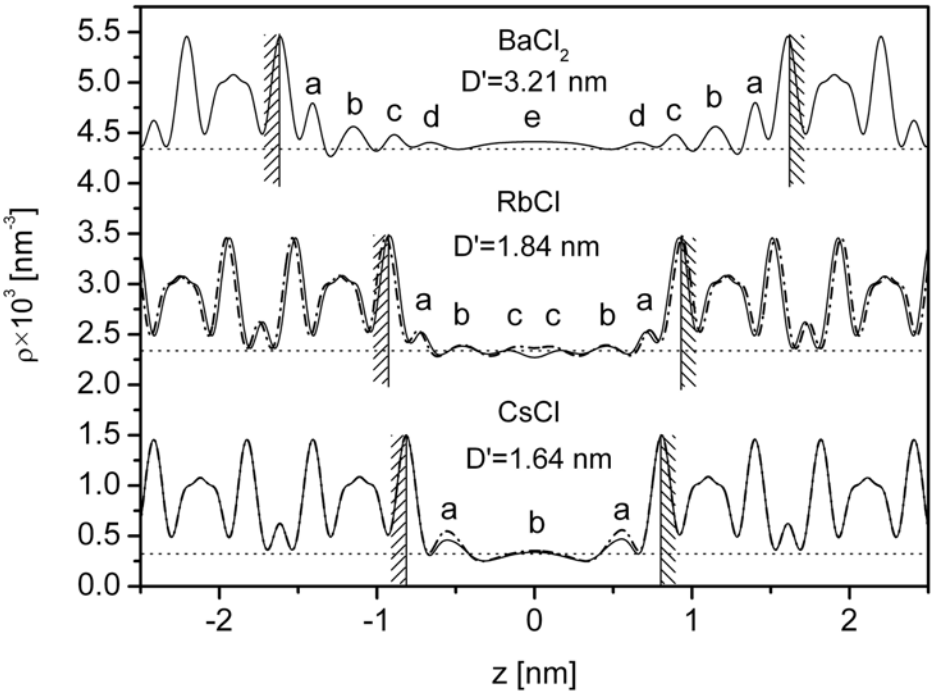
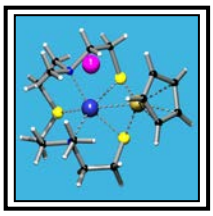


Fig. 2 Best-fit electron density profiles for confined RbCl at concentrations of 5.0 m and 7.5 m (up, baseline 4.0), BaCl2 at 11 m (center, baseline 2.0) and CsCl at 6.0 m and 11.0 m (down, baseline 0.0).

The Zürich School of Crystallography
Bring Your Own Crystals

University of Zürich
June 9 - 22, 2013



The fifth Zürich School of Crystallography took place, as usual, within the Institute of Organic Chemistry at the University of Zürich (UZH). The 19 enthusiastic participants from diverse corners of the world were inducted into the essential theory and practical aspects of small-molecule single-crystal X-ray crystallography. All aspects of the School ran very well with no hiccups and the enthusiasm of the participants remained high throughout, even though they find the School very intense. We maintained our usual 2:1 student:tutor ratio and participants always comment very favourably on the personalised friendly attention they receive. The participants this year comprised 1 MSc and 13 PhD students, 1 postdoc, 1 young academic, 2 more senior academics and 1 researcher. They came from 15 countries: Canada, Finland, Ghana, Italy, India, Nigeria, Poland, Romania, Slovenia, Switzerland, Sweden, Thailand, Turkey, The Ukraine and Uzbekistan; 8 women and 11 men, with ages ranging from 24 to 50. It is pleasing to see increasing interest from some African, Eastern European and Central Asian countries. The 10 tutors were from the Universities of Basel, Bern, Geneva, Zürich, the EPFL Lausanne, the ETH Zürich and the Institute of Physics, Prague.

The participants worked very hard throughout the School. The daily schedule of alternating lecture blocks and practical work in both the morning and afternoon sessions allows the participants to assimilate the theory and practical aspects readily. The practical work included hands-on experience in groups of two at one of the five diffractometers available in the various chemistry institutes at the UZH and ETH Zürich. The tutorial exercises and structure refinements were done in the computer classroom of the Institute of Organic Chemistry, UZH. We give the participants two real-case example data sets to cut their teeth on; they learn to use the software and to recognise and resolve unexpected difficulties with structures. Each participant then solved the structure of the compound they had provided crystals of in the lead-up to the School. In this way, they get excited about being able to solve the structure of a compound of specific interest to them. The supplied samples again provided a wide range of sample types (organic, organometallic, coordination polymer, natural product and mineral) and some interesting and demanding challenges, such as twinning, disorder, disordered solvent molecules, and unusual or ambiguous space groups. All participants were able to complete their structures successfully.

On the final day of the School, each participant gave a ten minute presentation on their own structure. Those desiring credit points had to sit a two-hour written exam while the remainder also took the exam to self-test their knowledge. Each day concluded with short discussion where participants can express their feelings about their experience that day. We also offer a repetition lecture slot where the topics can be nominated by participants who feel that they did not quite grasp a certain aspect the first time. Relaxation times and breaks benefited from the pleasant environment of the university campus and surrounds. Interesting discussions with the tutors often continued over the evening meal. Social events included a mixer, barbeque and a half-day excursion to the Swiss Light Source and SINQ neutron spallation facility of the Paul Scherrer Institute.

The central goal of the School is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination so that they could competently determine their own structures when they return to their home laboratory. With this in mind, the practical sessions and example structures are designed to allow the participants to see behind the button-pushing and learn about the actual procedures going on when various operations are performed, and then how to interpret whether or not the appropriate result has been obtained and other signs of success or unresolved problems.

At the end of the School, every participant completed a questionnaire. Very positive feedback was received about the quality of the School overall, the friendliness, accessibility and approachability of the tutors, the organisation, the venue and the accommodation. Participants often suggest including more example structures in the practical work, but course time is limited and already intense and we believe a balance of theory and practical work is important if the participants are to receive a proper understanding of the field. During the final banquet, each participant received a certificate and a copy of "Crystal Structure Refinement, A Crystallographer's Guide to SHELXL" by Peter Müller, kindly donated by the IUCr and OUP. After two weeks together, many new friendships had been established and people did not want to part company at the end of the last evening. The personal impressions of one of the participants are given further below. We are already planning for the next School, which will be held in June, 2015.

We are very grateful for the generosity of the sponsors: Institute of Organic Chemistry of the University of Zürich, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, International Union of Crystallography, Verlag Helvetica Chimica Acta, Oxford University Press, Agilent Technologies, Bruker AXS, Oxford Cryosystems and the X-ray Diffraction Services, CSEM, University of Neuchâtel, plus the support from the Chemistry Platform of the Swiss Academy of Sciences.

Tony Linden, Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2013 – Report from a participant

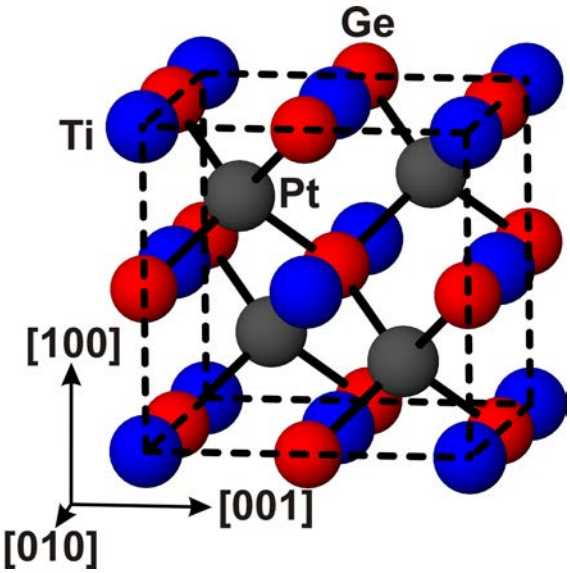
The 2013 Zürich School of Crystallography (ZSC) ran this June for 2 weeks (9-22 June) on the campus of the University of Zürich. This intense course is designed for senior graduate students or, in fact, anyone interested in learning the background and techniques of modern crystallographic characterisation of small molecules or intermetallics. This years' edition featured a very strong list of lecturers / tutors assembled by Tony Linden (Editor: *Acta Crystallographica C*; U. Zürich) and Hans-Beat Bürgi (Emeritus U. Bern / U. Zürich) which included H. Flack (Emeritus U. Geneva), J. Hauser, P. Macchi (both of U. Bern), G. Chapuis (Emeritus EPFL: Lausanne), O. Blacque (U. Zürich), M. Neuberger (U. Basel), L. Palatinus (Inst. Physics, Prague) and M. Wörle (ETH: Zürich). This potent collection of experts each lectured and tutored the participants who hailed from locations across Europe, Asia, Africa and North America. This course is designed for anyone wanting to expand their general knowledge of crystallography, experience first-hand diffractometer set-up and crystal mounting, to learn the various approaches to solving and publishing small molecule crystal structures and, perhaps most importantly, to be introduced to the various pitfalls and common errors which occur in crystal structure solutions. I've been involved with X-ray diffraction before, but had never solved a structure of my own, nor did I understand the meaning of much of the data commonly reported with X-ray diffraction data. The ZSC answered all of my queries and more. The course begins with an in-depth series of lectures on the background and applications of diffraction but quickly becomes a hands-on approach to crystallography. Perhaps the best thing was the opportunity to solve my own structure after learning the basics on provided, but real, datasets. However, it is not all lectures and computer work! We spent one afternoon visiting the Paul Scherrer Institute (www.psi.ch), home of Switzerland's Synchrotron facility. We were able to see and tour the complex instrumentation and meet a number of the scientists there who are involved in X-ray, neutron and related diffraction experiments. There was also plenty of time to socialize amongst the 19 participants and their 10 tutors with frequent coffee breaks, a barbeque, wind-down time over dinner and drinks and a concluding banquet. It was wonderful to meet and get to know all the other students from very wide backgrounds and from almost every corner of the world. I'm now back at home, but very keen to solve my next dataset. The ZSC certainly provided me with all the tools I need to solve crystal structures but it has also taught me what the common mistakes are and how to recognize them. The tutors and lecturers gave a thorough and informative overview of crystallography and gave me the tools I need to solve day-to-day datasets with confidence. As a participant myself, I would highly recommend this course for anyone wanting to expand their knowledge of the subject or as a refresher course for those who might want more cutting-edge instruction in modern crystallography.

Robert Gossage, Ryerson University, Toronto, Canada

Science coming out of the Zürich School of Crystallography

The recent paper in *Acta Crystallographica* B69, 457-464, *TiGePt - a study of Friedel differences* by Ackerbauer *et al*. (2013) is a product of the Zürich School of Crystallography held in June 2011. The objective of these two-yearly schools is to teach 20 young participants, mostly Ph.D. students, the basic notions of crystallography by a combination of lectures and practical classes in which each student solves their own crystal structure.

This study arose in a singular way. The crystal of TiGePt used for structure determination by Ackerbauer *et al*. (2012) (*Chem. Eur. J.* 18, 6272-6283) was submitted to the Zürich School of Crystallography [Linden & Bürgi (2008) *Acta Cryst.* A64, C30 and http://www.chem.uzh.ch/linden/zsc] by one of the 20 student-participants (S.-V. Ackerbauer) as her project study. Diffraction measurements (Mo *K*α radiation) were made by the school organizers and the student had to solve and refine the project structure, once two example structures provided by the school had been completed. The intermetallic compound TiGePt is atypical in its chemical composition and symmetry compared with most crystals submitted by the other student participants. At an *R* value of 1.1%, the study of TiGePt was still producing furrowed brows amongst the ten highly experienced tutors and the student. The values of statistics concerning the fit of Friedel opposites looked weird. In particular, it was not entirely clear whether the space group was non-centrosymmetric or not, and in the hustle and bustle of the school, there was no time to pursue these problems further. A lively e-mail discussion was undertaken following the school and its results are presented in the paper.



The X-ray single-crystal diffraction intensities of the intermetallic compound TiGePt were analysed. These showed beyond doubt that the crystal structure is non-centrosymmetric. The analysis revolves around the resonant-scattering contribution to differences in intensity between Friedel opposites *hkl* and $\bar{h}\bar{k}\bar{l}$. The following techniques were used: R_{merge} factors on the average (A) and difference (D) of Friedel opposites; statistical estimates of the resonant-scattering contribution to Friedel opposites; plots of $2A_{obs}$ against $2A_{model}$ and of D_{obs} against D_{model}; the antisymmetric D-Patterson function. Moreover it was possible to show that a non-standard atomic model was unnecessary to describe TiGePt. Two data sets were compared. That measured with Ag *K*α radiation at 295 K to a resolution of 1.25 $Å^{-1}$ is less conclusive for absolute-structure determination than the one measured with Mo *K*α radiation at 100 K to the lower resolution of 0.93 $Å^{-1}$.

Hans-Beat Bürgi, Howard Flack and Anthony Linden

Minutes of the General Assembly of the Swiss Society for Crystallography, held at Villa Olma in Como on 11.09.2013, during the MISSCA-2013 Conference.

The General assembly starts at ~17:35.

1. Jürg Schefer welcomes all members of the SGK, who have come for the General assembly in Como.

2. Jürg Schefer mentions, that in 2012, three members of the Society have passed away: Walter Petter, Gérald Bernardinelli and Jean Müller, and asks those present for a minute of remembrance

3. Formalities decided upon under the guidance of Jürg Schefer

- The invitation to participate to this General assembly has been sent out to all members in the Newsletter Nr. 88 (May, 2013), i.e. well in advance of the 21 days before the Meeting (as required by the Statutes);
- Denis Sheptyakov is asked to take the notes of the meeting, and agrees to do so;
- Delegates form the corporate members of the Society are being asked to identify themselves. Dubravka Šišak Jung from Dectris Ltd appears to be the only one representing the corporate members;
- Determination of the Quorum:

The number of participants is 19, herewith the quorum of 10% is fulfilled (as of August 2013, the Society comprises 169 individual and 10 corporate members), and the decisions of this General Assembly are legal and to be accepted by all the members of the Society.

4) Annual Report 2013:

4.1 Résumé of the activities:

- Annual meeting in Zürich organized by A. Linden, July 4-6, 2013
- Chaim Weizmann lecture in Fribourg, 23.04.2013, given by Prof. Dan Shechtman
- SSCr will organize the European Crystallography Meeting ECM-30 2016 in Basel, Switzerland August 28 to September 1, 2016
- Two newsletters published (Nr. 87 and 88)
- The Society has supported young scientists in terms of travel grants, poster prizes and financial support for the school of crystallography
- Completely new website with a modern design: http://www.sgk-sscr.ch/
- Webmanager: Celine Besnard, design Goetz Schuck
- 2 Board Meetings have taken place in Bern: 9. January 2013 and 5. July, 2013
- Participation in the MAP Meeting of the Academy of Science in Bern
- Forthcoming highlight: ScNAT Annual Meeting, 21/22 November 2013, Winterthur (Niels Bohr days)

4.2. Conferences and Courses supported by SGK/SSCr:

- Gordon Conference on Electron Distribution and Chemical Bonding, Les Diableret, July 2-12, 2013 (CHF 1500)
- The Crystallography School in Zurich, "Bring your own crystals", organized and hosted biennually by our members Tony Linden and Hans-Beat Bürgi at the Uni-ZH. 19 students participated, June (CHF 2000)

- Annual Meeting 2012 Zürich, ETH Hönggerberg (ScNAT contribution, CHF 3000 incl. poster prize)
- 3 travel grants were given to three young scientists in order to present their research at international conferences:
- S. Liuzzi (PSI)
- Y. Cheremond (Fribourg)
- D. Sisak (Zurich, June 2012)
- Support J. Schefer/K.Fromm, ECA-annual meeting, Warwick (reimbursed by ScNAT)

4.3 Membership statistics of the SGK – SSCr.

- 2012: 12 new members
- 2013: 7 new members, 7 exits
  losses mostly due by excluding the non-paying members
- Presently: 169 individual members
  10 corporate members

4.4 News from ECA/ECM-28

Highlight: ECM-28: European Conference in Warwick

Close to 900 participants, University Campus Warwick

- Main organizers: Sandy Blake and Elspeth Garman
- 7th Max Perutz Prize: Prof. Randy J. Read, Cambridge, for his contribution to the development and application of advanced statistical approaches to all stages of protein structure solution
- Opening Lecture: Prof. John Jenkin, Adelaide: History of the two Bragg's followed by several noon-sessions/events during lunch time
  "two Braggs Exhibition" with many original log-book entries, lab equipment, e.g.

5) Financial Report 2013

5.1. SCNat support in 2013 (Piero Macchi)

Jahrestagung	Organisation von Anlässen	2'500
Publikationen	Printprodukte zur Wissensverbreitung	0
Nachwuchsförderung	Organisation von Anlässen	500
Nachwuchsförderung	Reisekostenbeiträge an Dritte	1'500
Reise-und Werbungskosten	Organisation von Anlässen (inkl. 2'500 für ECM Bin in Warwick)	5'000
Mitglied ECA	Mitgliedschaft in international Unionen	120

5.2. Financial statement 2012 (Jahresrechnung 2012):

Total	31.12.2011	38'601.39
UBS account	31.12.2012	20'708.38
CS account	31.12.2012	18'016.72
Cash on hand	31.12.2012	653.50
Total	31.12.2012	39'378.60
Net income over the year (balance)		777.21

A Vote for acceptance of the Financial statement 2012 (Jahresrechung 2012):
Statement of the auditors: Approved: 26.3.2013 (Schenk/Bärlocher)

Request (Antrag):

Approval by the Annual Assembly / Entlastung Vorstand
(Approval, discharge of the Board)

The financial statement is being accepted unanimously.

6) Budget 2013

6.1. Proposal for the overall Budget:

Credits:	
Membership dues	5'000.00
SANW reimbursement for Annual Meeting 2013	3'000.00
SANW reimbursement for ECA delegate 2013	3'000.00
SANW young scientists travel grants	1'500.00
Interest (est.)	50.00
Total Income	12‘550.00
Debits:	
Membership dues to SANW (167 members)	1'200.00
Annual meeting	3'000.00
Travel Grant for ECA delegate (2013)	3'000.00
Travel Grants to Young Scientists	1'500.00
SGK support for Zurich School of Crystallography	2'000.00
Workshop at EPFL	1'000.00
ECA national membership dues 2013 (150€)	200.00
Bank charges	200.00
Total Expenses	12'100.00
Expected gain 2013	450.00

6.2. Finanzieller Jahresbericht 2013 – SCNat request for 2014

Jahrestagung (location to be selected by this assembly)	1'500
Publikationen	0
Nachwuchsförderung (Montreal-Delegation ECM30-Basel)	2'000
Nachwuchsfoerderung	1'500
Mitgliedschaft European Crystallographic Organisation ECA	140
Werbekosten Montreal 2014 (für ECM-30, Basel)	4'500
UN Jahr der Kristalloagraphie, Aktivitäten in CH	1'000

A vote: The proposed budget for 2013 with a gain of CHF 450.- is being accepted unanimously.

6.3. Hans-Beat Bürgi initiates a discussion:
The Society is rich and is accumulating the money further. We could consider two possibilities to spend the money: 1) SGK/SSCr prize for Young Scientists (for example, an SGK/SSCr medal and money on the order of CHF 1’000), or 2) invite prominent lecturer(s) to give lectures in several places in Switzerland
Piero Macchi:
1) The Society needs reserve for 2016, when the ECM will be hosted in Basel, for the case of significant financial losses, and 2) CHF 1’000 is not too much any way.
A discussion follows, with slightly differing opinions, Olha Sereda, Antonia Neels, Hans-Beat Bürgi, Piero Macchi and others are expressing their attention to the idea proposed by Hans-Beat Bürgi.

The final decision is that the Board will address this issue in its next meeting, and come up with corresponding decision(s).

6.4. Membership annual fee for the Year 2014:
The Board of the SGK/SSCr proposes to keep the membership fees as they are at the moment:
CHF 30.- for the regular members,
CHF 10.- for the students
CHS 130.- for companies (corporate members)
No alternative proposals are being done.
Voting for this proposal: also this initiative has been accepted unanimously.

6.5. Confirmation of the Board members and of the auditors.
6.5.1. The present Board of the Society:
C. Besnard
K. Fromm
M. Hennig
A. Linden
P. Macchi
A. Neels
J. Schefer
D. Sheptyakov
is being confirmed to continue its duties for the next year in a common vote unanimously.
6.5.2. The Auditors of the Society presently are: K. Schenk and C. Bärlocher.
C. Bärlocher (ETH Zürich) has asked the Society to find a replacement for him. Jürg Schefer has asked B. Spingler (University of Zürich) about his willingness to serve as an Auditor of the Society, and he has kindly agreed. The proposal of Jürg Schefer is herewith to vote for the following two Auditors of the Society for the Year 2014 onwards:
- Bernhard Spingler (University of Zürich),
- Kurt Schenk (EPF Lausanne)
The General Assembly votes unanimously to approve also this proposal.
Jürg Schefer wishes Bernhard Spingler all possible success in his new duty as an Auditor of the Society, and expresses his Gratitude to Christian Bärlocher for his long Service as an Auditor of the SGK/SSCr.
6.6. Jürg Schefer, who is presently also a delegate from the SGK/SSCr to the European Crystallographic Association, mentions that the Society also has to either confirm his delegation as such, or nominate a new delegate. Himself he proposes to consider Katharina Fromm (University of Fribourg) as a substitute for him. Anonymous voices from the Audience propose Jürg Schefer to continue his duties as a representative of the SGK/SSCr in this position. In its vote, the General Assembly confirms unanimously that Jürg Schefer will continue to represent the SGK/SSCr in the ECA.

7) Jürg Schefer informs the General Assembly about the activities of the SGK/SSCr and of its Board in connection with the forthcoming ECM-30 to be held in Basel, on 28.08-01.09.2016.
He lists the Activities in this frame:

28.08.2012	Olten	Kickoff-Meeting	Fromm/Schefer/ Hennig
10.12.2012	Basel	Meeting with the PCO, Congrex, Basel	Final reservation of the center, Messezentrum Basel, from Sunday Noon, 28.8.2016 to Thursday evening, Sept. 1, 2016
17.-18.2.2013	Budapest	Participation in the ECA Board meeting	Presentation of the contract with Congrex
08.01.2013	Fribourg/ Villigen	Contract with Congrex	Underwriting
05.06. 2013	Bern	SGK/SSCr Board meeting	Proposal for the local organizing committee
Aug. 2013	Warwick, ECM-28	ECA Counil	Report

Local Organizing Committee:

Katharina Fromm	University of Fribourg	confirmed
Jürg Schefer	PSI, Villigen	confirmed
Piero Macchi	University of Bern	confirmed
Anthony Linden	University of Zurich	confirmed
Denis Sheptyakov	PSI, Villigen	confirmed
Michael Hennig	La Roche, Basel	confirmed
Céline Besnard	University of Geneva	confirmed
Antonia Néels	CSEM Neuchâtel	confirmed
Walter Steuer	ETH Zürich	confirmed
Phil Pattison	EPF Lausanne	To be asked
Bernhard Spingler	University of Zürich	confirmed
Alex Dommann	EMPA St. Gallen	confirmed
Karl-Heinz Ernst	EMPA Dübendorf	To be asked
Markus Neuburger	University of Basel	To be asked
Tilman Schirmer	Biocenter Basel	confirmed on 11.10.2013

Jürg Schefer:
This list can be changed and is open for discussion
Present idea: board + broad local distribution

Anthony Linden:
We should start distributing the tasks and responsibilities within the local organizing Committee already now.
Jürg Schefer: Correct, we will organize a meeting of the local organizing Committee in the beginning of 2014 {Note in proof: The meeting of the Board will take place on 11.02.2014 in Basel}.

8) Varia.
8.1. Places and times for the next General Assemblies.
2014 – most probably in Neuchâtel, also under consideration was Basel.
Antonia Neels: Whether or not we will be able to host the Meeting at CSEM in Neuchâtel, will depend on the amount of the people we will be expecting to come. A meeting of up to ~100 people is fine with being hosted at CSEM.
2015 – A Board will contact EMPA in Dübendorf and also ask people in Genève and Lausanne.
2016 – either a Meeting is to be held as a satellite to the ECM-30, or it will be skipped (to be decided later).
8.2. Activities in connection with the forthcoming international Year of crystallography – 2014.

- Jürg Schefer demonstrates a poster from the exhitition „Voyage dans le cristal“ which he proposes to have demonstrated (upon being translated to German) in different Swiss Universities.
- Hans-Beat Bürgi indicated that he and Katharina Fromm have been asked to edit a special issue of "Chimia" devoted to the International Year of Crystallography 2014.

9. Other issues.

- Antonio Cervellino indicated that for the Powder Diffraction School at PSI, there is already sufficient financial support available, and that the School would rather appreciate if the Society could contribute to the advertisement of the School.
- Céline Besnard asks for the support (may be also – though very modest – financial) to the translation of the Posters from French into German.
- Michael Wörle (ETH Zürich) indicated that after a year of intensive discussions with the CSD, ETHZ has taken a decision that from now on, the ETHZ will pay the license fees for all of Switzerland. So that starting from now, everybody in the Swiss Universities can again have a full and unlimited access to the CSD. This news has been met with a joint excitement and applause. The SGK General Assembly expresses its gratitude to Michael Wörle and other people behind the negotiations with the CSD, as well as to the ETH at Zürich for this absolutely brilliant solution for all Swiss crystallographers.

The 2013 General Assembly oft he SGK/SSCr closed
at 18:20 on 11.09.2013 in Como.

MaMaSELF: Application for 2014-2016

Contributed by Jürg Schefer

MaMaSELF is a two year European Master program in Materials Science, which aims to teach the application of “Large Scale Facilities” for the characterization and development of materials.

Modern life and globalization imply new and additional exigencies for scientists and scientific engineers in the field of scientific and industrial competitiveness. This holds specifically for the development of new technologies and new materials which are important key-products and which contribute to the technological and scientific competitiveness of highly industrialized countries. The characterization of these materials and also the optimizing of technologies strongly demand sophisticated methods, some of them uniquely available at “Large Scale Facilities” using neutrons or synchrotron radiation.

The Master Course is supported by the European Commission in the framework of the Erasmus Mundus program.

Consortium: Rennes, Montpellier, Torino and Munich (TU, LMU)
Partners: ILL, FRM2, PSI, ESRF, LLB, DESY, Elletra and others.
Deadline For Both European And Non-European Students: 26 Jan. 2014
More information and on-line application: http://www.mamaself.eu

PAUL SCHERRER INSTITUT

PSI

Powder Diffraction School

Modern Synchrotron Methods

1–4 July 2014 • Paul Scherrer Institut • 5232 Villigen PSI • Switzerland

pds2014@psi .ch

Registration opens: January 2014

Speakers

To be announced.

Scope

The school aims to provide a general overview of modern synchrotron powder diffraction methods and their ever-increasing range of applications in materials science, chemistry, physics, life sciences and engineering.

Powder diffraction data provides a wealth of information, from determining the atomic structure of ordered and disordered materials, to investigating their detailed microstructure and their structural and microstructural response to external stimuli such as temperature, pressure, and external fields. Modern synchrotron techniques allow previously inaccessible in-situ experiments to be performed over a wide range of time scales.

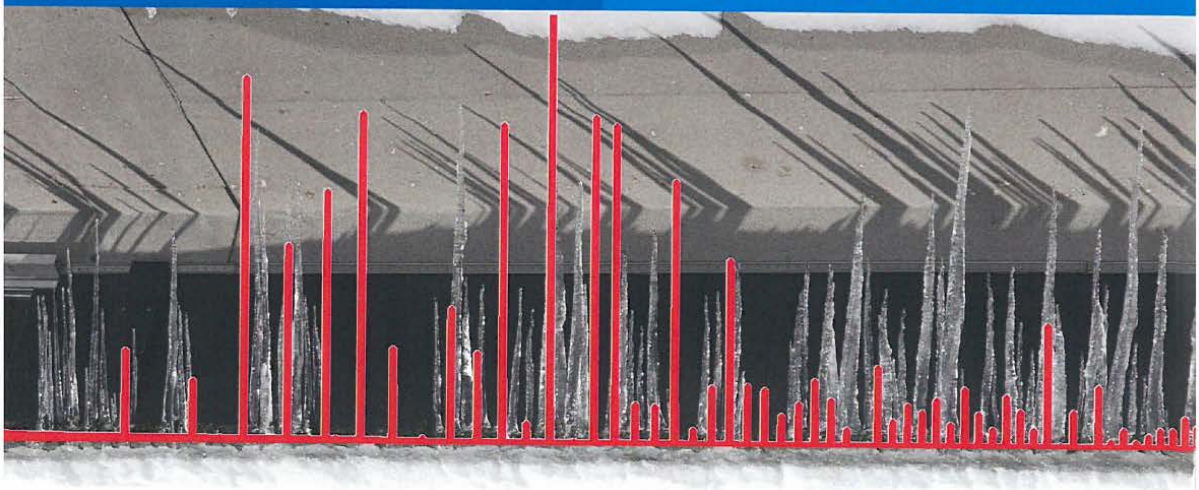
An in-depth program, starting with a general theoretical introduction to the various methods and applications, followed by hands-on practice with selected synchrotron XRPD experiments and by exhaustive analysis of the data so collected, will provide the student with a solid fundamental knowledge of this highly important and flexible experimental technique.

Organization

Antonio Cervellino
Nicola Casati
Martina Füglister (secretariat)

Topics

Atomic Structure Determination
Microstructure Analysis
Time-Resolved
Special and Advanced Topics



Croatian Association of Crystallographers
announces the workshop

HOT TOPICS IN CONTEMPORARY CRYSTALLOGRAPHY

Ministry of Science, Education and Sports of the Republic of Croatia

globtour event

AKD AGENCIJA ZA KOMERCIJALNU DJELATNOST

Solaris BEACH RESORT

Agilent Technologies

BRUKER

Molecular Dimensions

DECTRIS

PANalytical

RENACON

www.ccdc.cam.ac.uk

"Solaris" beach resort, Šibenik, Croatia
May, 10th - May 15th, 2014

Lecturers & some of their Hot Topics:

Hans-Beat Buergi (Bern): *The whole is more than sum of its parts*
Howard Flack (Geneve): *Absolute structure and absolute configuration*
Elspeth Garman (Oxford): *Triumph over Adversity: The structure determination of TBNAT*
Regine Herbst-Irmer (Goettingen): *Twinning in Crystallography*
Dietmar Stalke (Goettingen): *What a synthetic chemist learns from charge density?*
CCDC (Cambridge): *Advanced solutions from the CSD*

Application deadline: Feb, 1st, 2014

The workshop is designed and intended for PhD students, postdocs and young scientists, working and studying in scientific fields related to crystallography. Roughly 40% of the total working time of the Workshop will be dedicated to practical sessions and Q&A based discussions.The applicants are encouraged to present their own research results.
The organizing committee will cover all on-site expenses for the students.
For more, please visit

http://www.hazu.hr/kristalografi/HotTopics

Calls for proposals

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

Facility	Deadline(s)	Link
SLS: Swiss Light Source		www.psi.ch/useroffice
All except PX lines	March 15, Sept. 15	
Protein crystallography beamlines (PX)	Feb. 15, June 15, Oct. 15	
SINQ: Swiss Spallation Neutron Source		
All instruments (regular calls)	May 15, Nov. 15	www.psi.ch/useroffice
SINQ/SLS		www.psi.ch/useroffice
Joint powder instrument (MS/HRPT)	Feb. 15, 2014	
SμS: Swiss Muon Source		www.psi.ch/useroffice
All instruments	Dec. 5	
ESRF: European Synchrotron		
All instruments, long term proposals	Jan. 15	www.esrf.eu
All instruments, short term proposals	March 1, Sept. 1	www.esrf.eu
SNBL: Swiss Norwegian Beam Line	March 1, Sept. 1	www.esrf.eu/UsersAndScience/Experiments/CRG/BM01/
ILL: Institut Laue Langevin		
All instruments	Jan. 15, 2014	www.ill.eu
FRM II: Heinz Maier-Leibnitz		
All instruments	May 02, 2014	user.frm2.tum.de
SNS Spallation Neutron Source Oak Ridge	Feb. 26, 2014	neutrons.ornl.gov

Calendar of forthcoming meetings

(Please mail the missing information on meetings of interest to Jurg.Schefer@psi.ch)

			Abstract Deadline
2014			
Feb. 9-13	Perth Australia	Australian X-ray Analytical Association (AXAA) 2014 Workshops, Conference & Exhibition www.axaaconference.info	closed
Feb. 16-21	Guangzhou China	8th Int. Symposim Hydrogen & Energy http://hesymposium.ch	01.12.2013
Feb. 19-21	Grenoble France	NIBB 2014 "Neutrons in Biology and Biotechnology" http://www.ill.eu/nibb2014	10.01.2014
Mar. 17-20	Berlin Germany	Annual Conference of the German Crystallographic Society http://www.dgk-conference.de	12.12.2013
May 10-15	Šibenik Croatia	Workshop "*Hot Topics in Contemporary Crystallography*" http://www.hazu.hr/kristalografi/HotTopics/	01.02.2014
May 26-30	Lille France	E-MRS 2014 Spring Meeting, With 4 symposia in the category "Crystal Growth In Materials Science" http://www.emrs-strasbourg.com	16.01.2014
Jun. 1-5	Knoxville USA	2014 American Conference on Neutron Scattering (ACNS) http://www.mrs.org/acns-2014/	10.03.2014
Jun. 15-18	Aahrus Denmark	14th European Powder Diffraction Conference (EPDIC-14) http://epdic14.au.dk	15.03.2014
Aug. 5-12	Montreal Canada	IUCr-2014, 23rd General Assembly and Congress of IUCr http://www.iucr2014.org	11.02.2014
Aug. 28-Sep. 06	Pavia Italy	1*st* European Crystallography School 2014 http://2014.aicschool.org	to be announced
Sep. 1-5	Roskilde Denmark	35th Risø International Symposium on Materials Science http://www.dgm.de/dgm/mse-congress/	06.01.2014
Sep. 9	Neuchâtel CH	2014 Annual Meeting of the SGK / SSCr	to be announced
Sep. 23-25	Darmstadt Germany	Materials Science and Engineering (MSE 2014) http://www.dgm.de/dgm/mse-congress/	17.02.2014
Oct. 5-8	Ellwangen Germany	Summer school "*Theory and Practice of Modern Powder Diffraction*" http://www.kofo.mpg.de/iycr/index.html	to be announced
Oct. 5-14	Grindelwald CH	10th World Conference on Neutron Radiography (WCNR-10) http://indico.psi.ch/conferenceDisplay.py?confId=2019	03.03.2014
to be decided	Villigen CH	PSI Powder Diffraction Summer School	to be announced
2015			
Jun. 7-20	Zurich Switzerland	Zurich School of Crystallography – Bring Your Own Crystals	16.01.2015
Jun. 30 –Jul. 03	Lucerne Switzerland	5th European Pefc & H2 Forum http://www.efcf.com	to be announced
Jul. 1-4	Lucerne Switzerland	11th European SOFC & SOE Forum http://www.efcf.com	to be announced
To be fixed	Rovinj Croatia	ECM-29 2015 http://www.ecm29.org	to be announced
2016			
28. Aug-01. Sep	Basel CH	European Crystallographic Association, ECM-30 http://www.ecm30.org	to be announced

Become a member of SGK/SSCr

If you are working in the field of crystallography, you might be interested to become a member of our society. For more information as well as online registration, please go to our website (http://www.sgk-sscr.ch).
Presently, the yearly membership fee is CHF 30 (CHF 10 for students).

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

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

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

Signature: .....

Please FAX the completed form to: Denis Sheptyakov, +41 (0)56 310 2939
or use our online application form at http://www.sgk-sscr.ch
You may also use this form if you need to update your contact information.

Institutional members and supporting institutions

Corporate members

Stoe & CIE GmbH
Wissenschaftliche Instrumente

X-Ray Diffraction Services
CSEM, Neuchâtel

Supporting institutions

Member of the
Swiss Academy of Sciences

(If you would like to see your logo here, please contact our treasurer, Dr. Piero Macchi)

Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Societad Svizera per Cristallografia

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