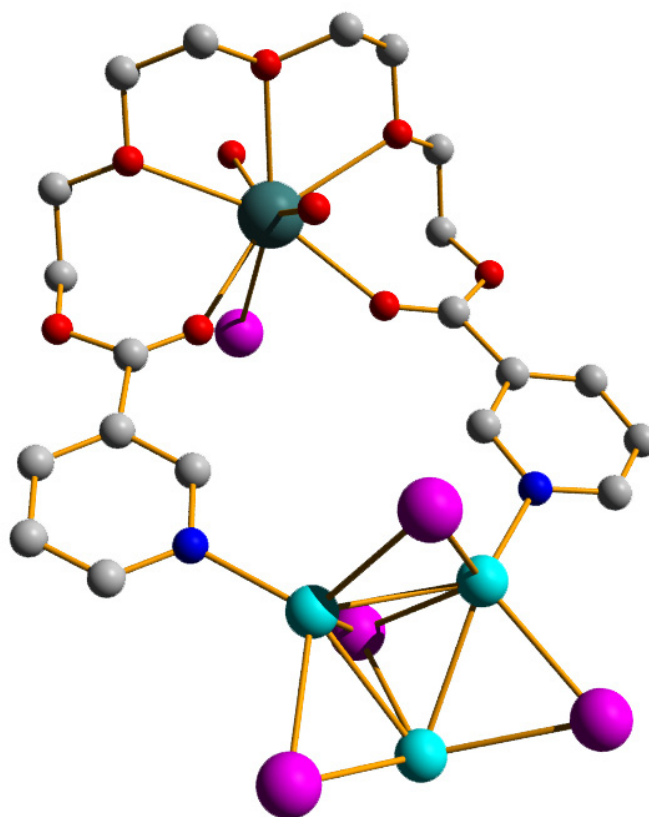


Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Swiss Society for Crystallography

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

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-  Mixed metal compounds for oxide materials
-  Program of the Joint Meeting of the SGK/SSCr and the National Center for Competence in Structural Biology, Sept. 8-9, Zurich
-  Agenda of the Annual General Assembly

On the Cover:

Complexes of alkaline earth and transition metal ions may provide precursors for the synthesis of high- T_c superconductors. The illustration on the cover shows $\text{CaCu}_3(\text{C}_{20}\text{H}_{24}\text{O}_7\text{N}_2)\text{I}_5(\text{H}_2\text{O})_2$. Report page 7

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I always enjoyed reading the letter of the president. However, this issue is missing his column, as it is not so easy to write a regular comment which is both, scientifically interesting and related to crystallography, but also amusing. I hope that you enjoy this 75th newsletter also without his column.

There are important meetings coming up: The 21st General Assembly of the IUCR in Osaka will be followed by our annual meeting at the University of Zurich (this year organized as a joint meeting together with the NCCR – the national competence center in research for structural biology). I hope you will attend both or at least one of these events.

Participants of the ECM-25 meeting in Istanbul should also note that this meeting has been delayed to August 16-21, 2009 due to the F1 grand prix taking place just before
....

Jürg Schefer
Editor SGK/SSCr Newsletter

Mixed metal compounds for oxide materials

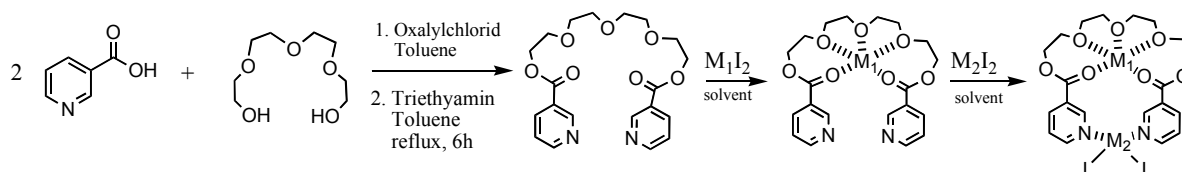
Contribution of Fabienne Gschwind and Katharina M. Fromm
University of Fribourg, Chemin du Musée 9, CH-1700 Fribourg, Switzerland

(will be presented also as a poster at the annual meeting in Zurich)

Introduction:

Complexes of alkaline earth and transition metal ions may provide precursors for the synthesis of high- T_c superconductors. Previous work has dealt with the synthesis of alkali and alkaline earth metal compounds, aiming among other properties also at the volatility of the products and their capacity of forming oxides [1]. We propose i) to make single source precursors with functional open polyether molecules, as well as ii) to use such compounds in new optical applications in nanotechnologies.

We developed a ligand system which allows the coordination to different metal ion types by different ligating atoms. With alkaline earth metal ions such as Ca^{2+} , the ligand wraps around the metal ion, yielding a complex in which the nitrogen atoms are oriented such as to accommodate very likely another, e.g. transition metal, ion.

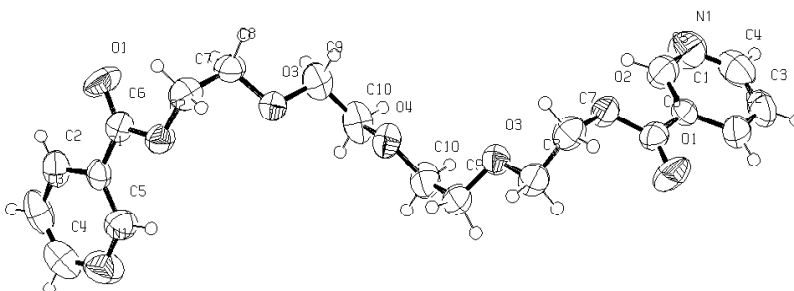


Results:

1) Ligand (L) [$\text{C}_{20} \text{H}_{24} \text{O}_7 \text{N}_2$]

We chose the ligand tetraethylene glycol bis nicotinic acid (L) for its potential to coordinate to two different metal ions for the generation of bimetallic species (Scheme1). Due to its quite long polyether chain, L can adopt different conformations and adapts therefore easily to any proposed metal ion.

This ligand can be synthesized in two steps.

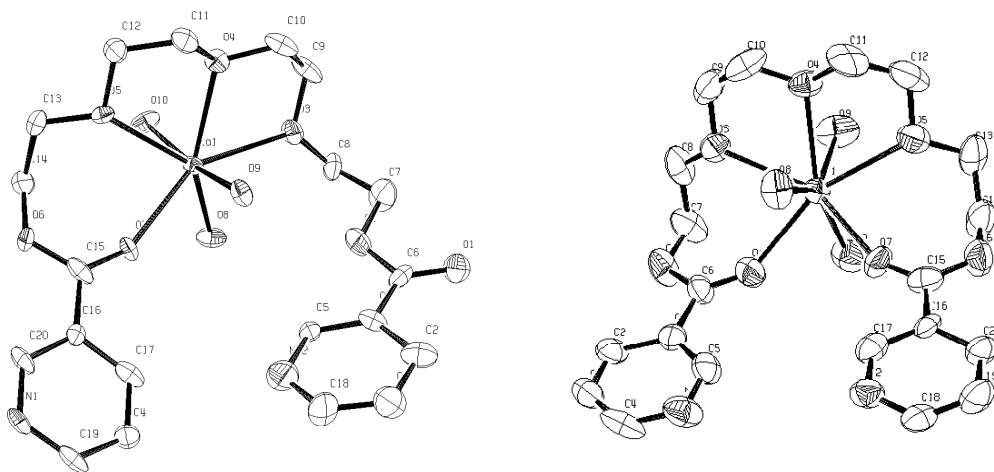


2) Monometallic complexes: Two isomers of $[\text{Ca}(\text{L})(\text{H}_2\text{O})_3]\text{I}_2$, **1** and **2**

We started to investigate the ligand **L** by studying its coordination behaviour to one metal ion type alone, M1 or M2. In the first case, we analyzed the complexation behaviour of the ligand **L** with Ca^{2+} -ions.

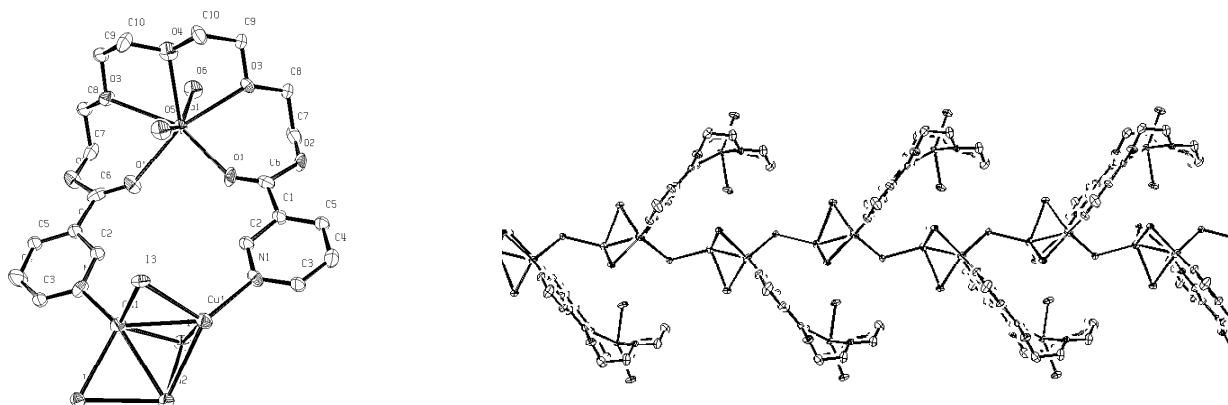
With CaI_2 , the ligand forms two different complexes under identical synthetic conditions. The first complex **1** crystallises in the monoclinic space group $P2_1/c$. The calcium ion is seven-coordinated, due to an "asymmetric" coordination of the ligand: one carbonyl group is pointing towards the calcium ion, the other one is pointing outside. The second complex of the same chemical composition is "symmetrically" built with both carbonyl groups pointing towards the metal ion. **2** crystallises in the monoclinic space group $P2_1/n$ and the calcium ion possesses an 8-coordination.

Repeated synthesis of the complexes, which are obtained under similar conditions, leads most frequently to the formation of **1**. This is possibly due to the fact that **2** has two rather strained metallacycles.



Bimetallic compound $[\text{CaCu}_3(\text{L})\text{I}_5(\text{H}_2\text{O})_2]$, **3**

Obtaining compound **3**, we reached the goal of a bimetallic compound by adding slowly CuI to a mixture of CaI_2 and **L** in chloroform. In the solid state, compound **3** crystallises in the orthorhombic space group $Pnma$. **3** presents a 1D-polymer structure in which the chain backbone is formed by Cu_3I_4 – cluster units linked via iodide ions. In contrast to **2** the calcium cation completes its coordination number of eight with two water molecules and one iodide.



Conclusions

A multitopic ligand approach for the synthesis of mixed metal compounds is described herein. With our ligand system it is possible to coordinate successively two different metal ions. Two calcium complexes, and a bimetallic compound were synthesised and fully characterised.

[1] K. M. Fromm, *Dalton Transactions*, **2006**, (43), 5103-5112.

News from Swiss-Norwegian Beamlines (SNBL)

Contribution of V. Dmitriev and P. Pattison

SNBL is now emerging from a period of refurbishment of the beamline infrastructure. This has included upgrading or replacing components such as vacuum controls, motor drives, electrical cables and, last but not least, a fresh coat of paint and a new floor covering. Despite the sometimes very dramatic disturbances to the normal operations of the beamtime (several kilometers of electrical cables were replaced, for example), we have been able to fit all refurbishment work into the regular shut-down periods of the ESRF. None of the scheduled experiments were disrupted, and we have been able to commission all of the new instrumentation without major problems. We are now optimistic that we can continue operation of the SNBL project for many years to come without major problems due to old and defective beamline components.

In addition to the improvements to the infrastructure of the beamline, we have also received some generous additional funds from the Swiss and Norwegian research councils which have enabled us to extend considerably the possibilities on the experimental stations. After some very successful trial experiments using Raman techniques in combination with diffraction and EXAFS measurements, we have now been able to purchase and install our own dedicated Raman spectrometer on the beamline. Fibre-optic connections to both experimental hutches allow us to collect in-situ Raman data under a wide variety of experimental conditions. In order to bring the new and exciting opportunities which this instrumentation provides to the attention of our user community, we have organized a SNBL workshop on the theme of combined

in-situ X-ray and Raman measurements. The workshop was held in Grenoble in June 2008, and was attended by about 80 participants. In order to reach out to a wider, international audience, we are pleased to announce that Taylor & Francis Ltd (London) will publish the SNBL Workshop Proceedings from our Raman meeting in a special issue of ***Phase Transitions***. This latest meeting followed on from earlier SNBL workshops on the themes of *Synchrotron Radiation in Studies of Nanoscaled Materials* and *In-situ experiments at SNBL using high gas pressures* held in 2006 and 2007, respectively.

It is widely accepted that modern synchrotron experiments often need a special sample environment in order to be able to investigate the behavior of materials ***in-situ*** and under something approaching "***real***" conditions. In this context, real conditions often imply extremes of temperature and pressure, or, for example, a sample contained within a special gas mixture. Examples of such research topics include the investigation of catalytic reactions or characterizing hydrogen storage materials during cycles of charging and discharging with hydrogen gas. After many years of building, and rebuilding, a series of ad-hoc control systems for regulating gas flow and mixing, we have now purchased a dedicated and tailor-made gas supply and mixing system which is fully computer-controlled. The availability of various micro reaction vessels permits the user to design his experiment in order to allow a reaction to take place under precisely controlled conditions. In addition, we have a portable mass-spectrometer which can be installed inside the hutch in order to characterize the gases produced during a catalytic reaction.

The last year or two has seen considerable improvements in the beamline configuration and the detector systems for EXAFS experiments. A new double-crystal monochromator has been designed, manufactured and commissioned by the beamline team. New EXAFS detectors have been purchased and improved electronics installed. The spectral range has been extended both to higher and lower energies, in order to be able to access a wider range of absorption edges. We will also shortly receive from PSI a small version of the very successful Mythen strip detector for powder diffraction experiments similar to the much larger detector currently installed on the SLS Materials Beamline. The availability of this detector will also extend the time-domain during which reactions can be studied. Our present powder measurements are either performed in scanning mode (which is inherently slow) or else with the mar345 image plate (where the detector read-out time is a handicap). The very fast read-out cycle of the Mythen strip detector will extend our temporal resolution for powder diffraction measurements into the sub-second domain.

With an eye towards the medium-term development of SNBL, the SNX Council has appointed a committee to consider the options and priorities for the beamtime in the time-frame of the present 4-year funding period and beyond. This committee is now collecting comments and suggestions from the synchrotron user communities in Norway and Switzerland, and is due to report back at the end of 2008.

News for and from members

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

Personal members

Dr. Götz Schuck

(Spallation Neutron Source Division, Paul Scherrer Institut, WBBA-115, CH-5232 Villigen PSI, Switzerland)

Dan Xie

(Laboratory for Crystallography, ETH Zürich, HCI G 504, Wolfgang Pauli Strasse 10, CH-8093 Zürich, ph.D. student)

Dr. L. Pernot

(University de Genève, Fac. Pharmacy, Quai Ernest Ansermet 30, 1211 Genève)

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.

Details for applications are given at:

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

Pending Membership Fees

We would like to thank (most of you) for the prompt payment of the 2008 membership fee.

However, several of the fees for 2008 and even a few back to 2006 are still missing. The cover letter indicates the **total amount due** (a negative balance means that you paid in advance and no action is needed).

Please pay the amount due immediately **by bank transfer** to the UBS account: IBAN CH39 0027 9279 C029 1110 0 , BIC: UBSWCHZH80A

Please avoid to pay in cash at a post office (PC 80-2-2, UBS Zürich, Account No. 230-C0291110.0) as Postfinance is charging handling fees to the society.

Thank you for your cooperation.

Your treasurer,
Michael Hennig

Annual Meeting of the SGK/SSCr at the University of Zurich, September 8-9, 2008

Joint meeting of the SGK and the National Center of Competence in Research for Structural Biology

Location

Main Building University of Zürich City (detailed map on page 32)
Lecture Hall KOH B10
between Künstlergasse and Rämistrasse

Scope of the Meeting

- Bring together the national center of competence in research 'structural biology' and Swiss society for crystallography
- Use the annual meeting of both organizations for a joint meeting
- Majority of lectures organized by the NCCR, one afternoon with lectures focused to more crystallographic topics followed by the annual general meeting of the SGK

Registration:

Until **Aug. 29, 2008** at <http://www.structuralbiology.uzh.ch/symposium2008.asp>
Further information: Dr. Patrick Sticher Moser

Conference Dinner SGK/SSCr

Tuesday, Sept. 9, 2008, time: 19h, Place: Restaurant Linde Oberstrass,
Universitätstrasse 91, 8006 Zürich (Tram 10, <http://www.linde-oberstrass.ch>)
Registration mandatory: cornelia.aurelio@mat.ethz.ch

Organizing committee:

(*) Posters (format A0 portrait) on any crystallographic subject may be presented during the whole meeting.

Detailed meeting information and abstract template
<http://www.sgk-sscr.ch>

Program of the Joint NCCR/SGK/SSCr Meeting

Day 1

September 8, 2008		
	NCCR Symposium	
09:00		Registration Welcome coffee
10:00	Markus Grütter NCCR Director	Welcome address
10:15	Poul Nissen University of Århus, Denmark	The structure and function of P-type ATPase cation pumps
11:15	Kaspar Locher ETH Zurich and NCCR Structural Biology, Zurich	Structure and mechanism of ABC transporters
12:15		Lunch and poster viewing
13:45	Titia Sixma The Netherlands Cancer Institute, Amsterdam	Protein-protein interactions regulating SUMO and ubiquitin conjugation
14:45		Coffee and poster viewing
15:30	Jeffrey Skolnick Georgia Institute of Technology, Atlanta	A structural proteomics approach to inference of protein function
16:30	Andrej Sali University of California San Francisco	Integrating diverse data for structure determination of macromolecular assemblies

Day 2

September 9, 2008		
08:15		Morning coffee and poster viewing
09:15	A. Joshua Wand University of Pennsylvania, Philadelphia	Adventures in NMR spectroscopy of encapsulated proteins dissolved in low viscosity fluids
10:15		Coffee and poster viewing
10:45	Stephen Kowalczykowski University of California Davis	DNA motor proteins: Structure and single-molecule visualization
11:45	Keiichi Namba University of Osaka, Japan	Molecular mechanisms of self-assembly and protein export of the bacterial flagellum
12:45		Lunch and poster viewing
13:45	Ilme Schlichting Max Planck Institute for Medical Research, Heidelberg	When flavins get the blues
14:45	Markus G. Grütter University of Zurich and NCCR Structural Biology, Zurich	Chaperone-assisted crystallography with soluble and membrane proteins
15:45		Power break
		Annual Meeting of the Swiss Society for Crystallography (SSC)
16:05	Michael Hennig Swiss Society for Crystallography	Welcome note
	Clemens Schulze-Briese Swiss Light Source at the Paul Scherrer Institute, Villigen, Switzerland	PILATUS 6M - protein crystallography with 6 million detectors
	Colin Nave Diamond Light Source, Didcot, UK	Potential of synchrotrons and free electron lasers for collecting x-ray data from very small samples
	Timothy J. Richmond NCCR Deputy Director	Concluding Remarks

Agenda of the SGK/SSCr General Assembly 2008

September 9, 2008, room KOH-B10 at 17:30h
University of Zurich, City Campus

- 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) Wahlen: Keine
- f) Anträge von Mitgliedern

Conference Dinner SGK/SSCr

Tuesday, Sept. 9, 2008, time: 19h, Place: Restaurant Linde Oberstrass,
Universitätstrasse 91, 8006 Zürich (Tram 10, <http://www.linde-oberstrass.ch>)

Registration for the dinner: cornelia.aurelio@mat.ethz.ch

Abstracts

Lectures

New opportunities in macromolecular crystallography : the PILATUS 6M pixel detector

Clemens Schulze-Briese¹, Ch. Brönnimann^{1,2}, E.F. Eikenberry², H. Billich¹, C. Rajendran¹, J. Diez¹, V. Olieric¹, B. Henrich¹, M. Kobas¹, M. Näf^{1,2}, E. Panepucci¹ and T. Tomizaki¹

¹ Swiss Light Source at PSI, CH-5232 Villigen PSI, Switzerland

² DECTRIS Ltd., CH-5232 Villigen PSI, Switzerland

The PILATUS 6M, developed at PSI, is the first large area pixel detector which is routinely operated at a protein crystallography beamline. It combines the data accuracy of counting detectors, with very high count rate capabilities on both the pixel and the detector levels. In addition it exhibits an excellent point-spread-function, and supports frame rates of up to 12.5 Hz allowing continuous shutter-free data acquisition and fine-phi slicing.

The integration of the detector into the beamline as well as the necessary changes to the computing environment and the data processing software will be discussed. Crystallographic advances and new opportunities in macromolecular crystallography made possible by the excellent performance of the detector will be presented. Future prospects for the use of the pixel detector in the collection of diffuse scattering from protein crystals will be discussed.

Potential of synchrotrons and free electron lasers for collecting x-ray data from very small samples

Colin Nave¹ and John A. Cowan²

¹ Diamond Light Source Ltd., Diamond House,

Harwell Science and Innovation Campus, Didcot, Oxfordshire, O11 0DE, UK

² STFC Daresbury Laboratory, Daresbury, Warrington, Cheshire, WA4 4AD, UK

There are plans in Switzerland and elsewhere to build x-ray free electron laser sources to provide pulsed coherent x-rays to supplement the already bright radiation from 3rd generation synchrotron sources. One of the aims of both synchrotron and free electron laser sources is to examine smaller and smaller samples. Examples in the field of life sciences include small protein crystals (sometimes only one unit cell!) and biological cells. One of the main issues, especially for biological samples sensitive to radiation damage, is to maximize the scattering/diffraction while minimizing the dose deposited in the sample.

For synchrotron sources, the possibility of reduced radiation damage for small crystals (10nm and below in size) under the conditions where the photo-electrons could escape the sample was examined some time ago [1]. The conclusion was that higher energy

radiation (e.g. 40keV) could offer an advantage as the photo-electron path length was greater and less energy would be deposited in the crystal. These calculations have now been extended [2] by including the effects of energy deposited due to Compton scattering and the energy difference between the incident photon and the emitted photo-electron. This allows an estimate to be made for the optimum wavelength for collecting data from a protein crystal of a given size and composition and the reduced radiation damage which could occur while doing this. The conclusions should also be relevant for examining other small samples such as the structure determination of biological cells by coherent diffraction.

Another way of reducing radiation damage, relevant to x-ray free electron laser sources, is to collect data with a very short pulse of x-rays so that a single image can be obtained before subsequent radiation damage occurs. A comparison of this approach compared with the use of shorter wavelengths on a synchrotron source will be made.

[1] Nave, C. & Hill, M. (2005). *J. Synchrotron Rad.* 12, 299-303

[2] Cowan, J. A. & Nave, C. (2008) *J. Synchrotron Rad.* In press

Posters

In-situ synchrotron powder diffraction study of hydrolysis of light hydrides

Elena Gobechiya,^{1*} Klaus Yvon,¹ and Yaroslav Filinchuk^{2*}

¹ Laboratory of Crystallography, University of Geneva, Switzerland

² Swiss-Norwegian Beam Lines at ESRF, Grenoble, France

Light metal hydrides are considered as possible hydrogen carriers for future mobile applications. One way to liberate hydrogen is by reaction with water. Hydrolysis of some light hydrides, e.g. borohydrides LiBH_4 , NaBH_4 and alanates LiAlH_4 , NaAlH_4 , has already been studied in some details [1], and it was shown that the reaction often does not proceed to completion. The reasons of this behavior are unknown, usually being attributed to a passivation of the hydride surface or a formation of intermediate phases. In-situ diffraction experiments allow following the evolution of the crystalline phases during hydrolysis and thus may shed some light on the reaction mechanisms in hydride- H_2O systems.

Here we report on the in-situ synchrotron powder diffraction study of the hydrolysis of NaBH_4 , $\text{Mg}(\text{BH}_4)_2$, LiAlH_4 , NaAlH_4 , $\alpha\text{-AlH}_3$, NaMgH_3 , and $\text{Ca}_4\text{Mg}_3\text{H}_{14}$. MAR345 area detector at SNBL-A provided 2 min time resolution and high quality data. This allowed to detect intermediate crystalline phases and determine their crystal structures. Three different setups were used, where hydrides were allowed to react with 1) air humidity; 2) water vapor brought by a stream of wet nitrogen gas; 3) a droplet of water placed in a direct contact with the sample or in a close proximity to it. To influence the kinetics, the reaction volume was cooled or heated.

$\alpha\text{-AlH}_3$ reacts with water and water vapor without formation of intermediate phases, yielding $\text{Al}(\text{OH})_3$. Under the same conditions $\text{Mg}(\text{BH}_4)_2$ gives an amorphous phase as a final reaction product. Amorphous phases form only as intermediates in the hydrolysis of LiAlH_4 , NaAlH_4 , NaMgH_3 and $\text{Ca}_4\text{Mg}_3\text{H}_{14}$. The final products are: $\text{LiAl}_2(\text{OH})_7 \cdot 2\text{H}_2\text{O}$ for the reaction of LiAlH_4 with water; $\text{Al}(\text{OH})_3$ for the reaction of NaAlH_4 with water and water vapor; $\text{Mg}(\text{OH})_2$ for the reaction of NaMgH_3 with water and water vapor; and $\text{Ca}(\text{OH})_2$ for $\text{Ca}_4\text{Mg}_3\text{H}_{14}$. Some of the investigated hydrides (LiAlH_4 , NaAlH_4 , NaMgH_3) are very reactive. On contact with air they react with atmospheric CO_2 and form carbonates: Na_2CO_3 and $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ in case of NaMgH_3 and LiAlH_4 , and Li_2CO_3 in the case of LiAlH_4 . $\text{LiOH} \cdot \text{H}_2\text{O}$ forms as an intermediate in the reaction of LiAlH_4 with water at lower temperatures (3°C). NaBH_4 is the most stable with respect to hydrolysis: in the reaction with water or water vapor below 40°C it yields only the hydrate $\text{NaBH}_4 \cdot 2\text{H}_2\text{O}$ [2], while at higher practical temperatures ($<100^\circ\text{C}$) the H_2 release is very slow.

- [1] R. Aiello, J.H. Sharp and M.A. Matthews, Int. J. Hydrogen Energy, **24**, 1123 (1999).
[2] Y. Filinchuk, H. Hagemann, Eur. J. Inorg. Chem., 3127 (2008).

Local order of deuterium in Laves phase deuterides

Joanna Ropka¹, Radovan Černý¹, Valérie Paul-Boncour² and Michel Latroche²

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² CMTR, ICMPE, CNRS, 2 rue H. Dunant, 94320 Thiais Cedex, France

The deuterides of cubic (C15) Laves phases have been widely studied for the influence of deuterium absorption on their magnetic properties. The systems YFe_2D_x and YMn_2D_x are particularly interesting due to the large variety of crystal structures depending on the D content. When absorbing deuterium the metallic matrix retains the cubic cell ($Fd\bar{3}m$) above the deuterium ordering temperature. Below this temperature the symmetry is lowered and a fully ordered coordination of metals by deuterium atoms is obtained in the deuterium rich phases. Little is known about the local deuterium configuration around the transition metal atoms in the disordered phase even if a considerable amount of diffuse intensity was reported in the neutron powder patterns (Figure 1).

Analysis of YFe_2D_x and YMn_2D_x by Pair Distribution Function (PDF) will be presented. Neutron Time-of-Flight data were collected at IPNS, Argonne, and Lujan Center, Los Alamos on series of samples with different deuterium content. Each sample was measured below and above the temperature of deuterium ordering. The PDF in ordered and disordered states look very similar up to the radial distance of $\sim 8 \text{ \AA}$, which is comparable with the lattice parameter of a cubic Laves phase deuteride. The observed PDF was modeled in the disordered state using the same local model as in the ordered phase (Figure 2).

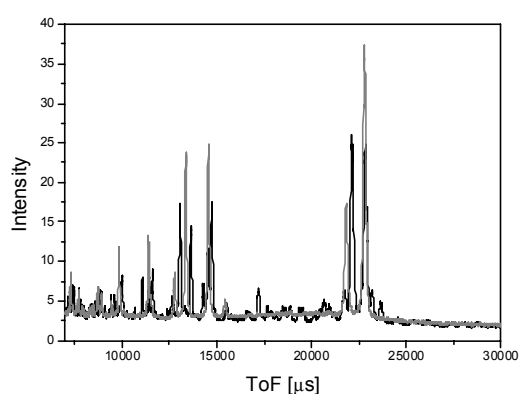


Figure 1. Observed neutron Time-of-Flight powder patterns of $\text{YFe}_2\text{D}_{4.2}$ in deuterium disordered (gray) and ordered (black) state. Note the diffuse intensity in the disordered state.

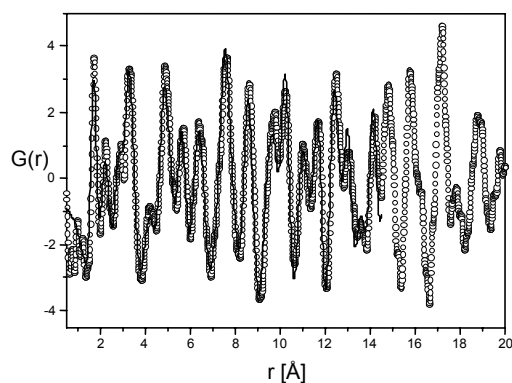


Figure 2. Observed Pair Distribution Function (points) of $\text{YFe}_2\text{D}_{4.2}$ in disordered state: Modelling (solid line) by same local order of deuterium atoms around iron as in ordered phase.

KSm(MoO₄)₂, an incommensurately modulated and partially disordered structure of the (3+1)D scheelite structure type

Alla Arakcheeva¹, Philip Pattison^{1,2}, Gervais Chapuis¹, Vladimir Morozov³,
Marta Rossell⁴ and Gustaaf Van Tendeloo⁴

¹ École Polytechnique Fédérale de Lausanne, Laboratoire de cristallographie, BSP,
CH-1015 Lausanne, Switzerland

² Swiss-Norwegian Beamline, ESRF, BP-220, F-38043 Grenoble Cedex, France,

³ Department of Chemistry, Moscow State University, 119899 Moscow, Russia

⁴ EMAT, University of Antwerp, Groenenborgerlaan 171, B-2020, Antwerp, Belgium

The incommensurately modulated KSm(MoO₄)₂ structure belongs to the (3+1)D scheelite structure type. It has been refined in the monoclinic superspace group $I2/b(\alpha\beta)00$ by the Rietveld method on the basis of synchrotron radiation powder diffraction data [1]. The systematic broadening of satellite reflections has been accounted for by applying anisotropic microstrain line-broadening [2]. The microstructure has been studied by transmission electron microscopy (TEM). The partial disorder of the K and Sm cations in the *A* position is best approximated by a combination of harmonic and complex crenel functions with (0.952 Sm + 0.048 K) and (0.952 K + 0.048 Sm) atomic domains. This combination yields a compositional wave distribution from {KMoO₄} to {SmMoO₄} observed in the *ab* structure projection along *q*.

Investigation of incommensurately modulated KSm(MoO₄)₂ structure confirms the (3+d)D structure type concept [3]. The (3+1)D scheelite structure type is characterized by superspace group $I2/b(\alpha\beta)00$. The basic unit cell contains two building units, *A* and *XO₄*, both occupying 4*e* Wyckoff site, *A* [4*e*: 1/2 1/4 *z_A* ≈ 0.88] and *X* [4*e*: 1/2 1/4 *z_X* ≈ 0.5]. In this structure type, the occupation and displacive atomic modulations along with coefficients of the vector *q* are variables. The complex occupation function of *A* position revealed in KSm(MoO₄)₂ structure for K and Sm along with different crenel functions allows to describe the full spectrum of the known compounds belonging to the (3+1)D scheelite structure type [3].

[1] Arakcheeva, A., Pattison, Ph., Chapuis, G., Rossell, M., Filaretov, A., Morozov, V. and Van Tendeloo, G. (2008) *Acta Cryst.* B64, 160-171.

[2] Leineweber, A. and Petříček, V. (2007). *J. Appl. Cryst.* 40, 1027-1034.

[3] Arakcheeva, A. and Chapuis, G. (2008) *Acta Cryst.* B64, 12-25.

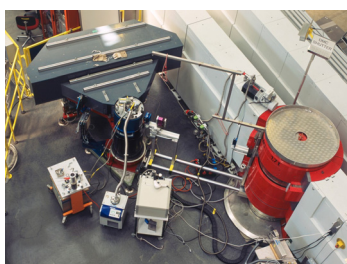
Neutron diffraction at the continuous spallation neutron source SINQ – The neutron diffractometers HRPT, DMC and TriCS

L. Keller, V. Pomjakushin, J. Schefer, D. Sheptyakov, V. Sikolenko, O. Zaharko

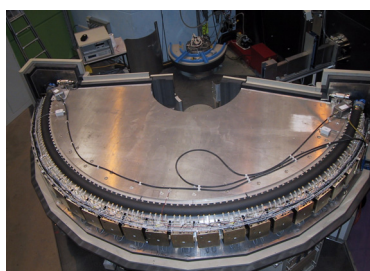
Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institut,
5232 Villigen PSI

We present the performance and the possibilities on the three diffraction instruments (single crystal diffractometer, TriCS, and the two powder diffractometers, HRPT and DMC) operated by the neutron diffraction group and give an outlook on the future instrumentation: Our replacement program just started with the new DMC-II powder diffractometer, which includes a two-dimensional position sensitive detector (expected to be operational 2012) and will continue with the single crystal diffractometer, where we are presently defining the parameters of the instrument: For example the maximal field at the sample position will reach 15 Tesla on such a new instrument.

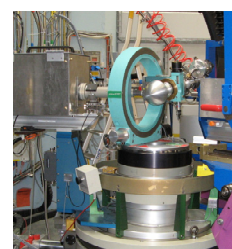
DMC [1]
Powders, low q



HRPT [2]
Powders, high-q



TriCS [3]
Single crystals



λ [Å]	2.3-4.2-(6)	1.15-2.41	1.18, 2.31
Temperature	50mK-2000K	50mK-2000K	4.2-600K
Pressure	100kbar	100kbar	25kbar
Max. Field	4 Tesla vertical 2 Tesla horizontal	4 Tesla vertical 2 Tesla horizontal	4 Tesla vertical 2 Tesla horizontal
Minimal sample	> 100-200mg	100mg	20mg
Detector	BF ₃ , PSD 80°	He ³ , PSD 160°	He ³ , single +2D

The powder diffractometers DMC having a very good resolution at low q is mostly designed for investigations of magnetic structures, whereas HRPT with its extended q-range allows high-resolution investigations of nuclear- and magnetic structures. TriCS is completing the possibilities for single crystal investigations.

SINQ provides an excellent sample environment, ranging from high pressure, high field, very low and very high temperatures to specialties such as in-situ measurements under hydrogen gas or light-illumination.

A central new development is presently on its way: The new 2D-detector presently under design will not only increase the intensity of DMC, but also allow mapping of magnetic reflections from single crystals.

- [1] P. Fischer, L. Keller et al,
Neutron News 11, No 3, 19-21 (2000), <http://sinq.web.psi.ch/dmc>
- [2] P. Fischer et al., Physica B **276-278**, 146 (2000), <http://sinq.web.psi.ch/hrpt>
- [3] J. Schefer et al., Physica B **276-278** 168-169 (2000) , <http://trics.web.psi.ch>

Uranyl mediated photocleavage in proteins

Annasara Dahlström, and Marc Schiltz

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Uranyl ions absorb light in the UV-visible region and have been found to bind to and cause photo-cleavage in biomolecules such as proteins and nucleic acids. In DNA, the uranyl ion binds to the phosphate backbone of the molecule and can potentially cleave the molecule between any base pair along the chain. In proteins, this binding and thereby the induced structural changes, are much more specific. One of many uranyl-binding proteins is porcine pancreatic elastase (PPE).

In this study, elastase-crystals have been soaked in a uranyl-containing buffer and several data sets have been collected in house and at the synchrotron at both room temperature and at 100K. The uranyl binds with high occupancy in a single position close to the well-known calcium/sodium binding-site. Only small conformational changes compared to the native structure are seen upon ligand binding. These changes originate from amino acids moving either to accommodate space for (Tyr71) or to coordinate the ligand (Glu59, Glu69). However, the sodium ion is not moving from its native site. In addition, two acetates bind to the uranyl.

After irradiation (400nm, 2h), the observed structure is still that of the native structure. However, the density of one amino acids in the direct proximity of the uranyl ion, Asn63, has completely disappeared. The densities of the acetates have also degraded and only the positions of the coordinating oxygens are visible.

Duff Jr, M. R., Kumar, C.V., Site-selective photocleavage of proteins by uranyl ions. *Angewandte Chemie –International Edition* **2006**, 45, 137-139.

Nielsen, P.E., Jeppesen, C., Buchardt, O., Uranyl salts as photochemical agents for cleavage of DNA and probing of protein-DNA contacts. *FEBS Letters* **1988**, 235, 122-124.

Combining X-ray powder diffraction and electron microscopy to solve complex structures

Dan Xie, Christian Baerlocher and Lynne B. McCusker

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When a complex structure of a polycrystalline material cannot be solved from X-ray powder diffraction (XPD) or electron microscopy data alone, combining the two techniques might succeed. Phase information derived from high-resolution transmission electron microscopy (HRTEM) images can be combined with XPD intensities to facilitate structure solution. Alternatively, the single-crystal intensities from electron diffraction (ED) data can be used to improve the estimate of the relative intensities of reflections that overlap in the XPD pattern. The first approach has already proven to be a powerful one [1,2], but it requires HRTEM images, which are not always easy to obtain. The second is the subject here.

Tests show that intensities from conventional selected area electron diffraction patterns are not very reliable because of multiple scattering effects, so they cannot be used directly to repartition the intensities of overlapping reflections. However, the precession electron diffraction (PED) technique [3] reduces these effects. The PED intensities are still distorted, so we took a very conservative approach, using them simply to identify the weak reflections. These reflections were then eliminated from the XPD intensity extraction. Initial tests of the feasibility of this approach were performed on the zeolite ZSM-5 using the powder charge flipping (pCF) program [4] and simulated ED patterns along 3 zone axes. Then real PED data were used. In both cases, the final pCF electron density maps revealed the positions of all 12 Si and 26 O atoms in the framework structure. This is not the case when the original XPD data without weak reflection elimination are used. It appears that even this simple modification of the dataset has a significant impact on structure solution.

[1] Gramm F et al. (2006) *Nature* **444**, 79

[2] Baerlocher Ch et al. (2007) *Science* **315**, 1113

[3] Vincent R, Midgley PA (1994) *Ultramicroscopy* **53**, 271

[4] Baerlocher Ch, McCusker LB, Palatinus L (2007) *Z. Kristallogr.* **222** 47

Designing PET tracers for HSV1-TK-based gene therapy using structural biology and molecular dynamics

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Therapeutically efficient nucleoside analogues against Herpes Simplex Virus 1 are selectively activated via its Thymidine Kinase (HSV1-TK). Further metabolized to triphosphates, they inhibit viral replication by blocking the viral DNA-polymerase. Being trapped inside the cell due to their negative charges, they are suitable for Positron Emission Tomography (PET) to monitor HSV1-TK activity *in situ*.

Previous biochemical and structural studies have shown that pyrimidine derivatives with a side-chain attached to the C-6 of the pyrimidine ring (alkylated side-chain) display good binding affinities for HSV-1 TK and no cytotoxic effects [1-2]. These findings gave a first indication that C-6 alkylated pyrimidine derivatives might find application as new non-toxic PET-tracer molecules which are specifically and efficiently phosphorylated by the HSV-1 TK.

Here, we present the structure of HSV1-TK at 2.0 Å complexed with a C-6 alkylated pyrimidine derivative, namely N-Methyl-DHBT (N-Methyl-6-(1,3-dihydroxy-isobutyl) thymine) as well as molecular dynamics to design PET tracers for HSV1-TK-based gene therapy. With dynamics, we assess the stability of HSV1-TK regions allowing binding of experimentally determined high affinity substrates and spot more flexible regions where substitutions could be beneficial. To this end, 3 different high resolution crystal structures of HSV1-TK in complex with their respective substrates have been simulated with NAMD 2.6 [3]. Subsequently, first substitutions possibly improving the binding affinity are pointed out.

- [1] Raic-Malic S, Johayem A, Ametamey SM, Batinac S, De Clercq E, Folkers G, Scapozza L. Synthesis, 18F-radiolabelling and biological evaluations of C-6 alkylated pyrimidine nucleoside analogues. *Nucleosides Nucleotides Nucleic Acids*. **2004**;23(11):1707-21
- [2] Johayem A, Raic-Malic S, Lazzati K, Schubiger PA, Scapozza L, Ametamey SM. Synthesis and characterization of a C6 nucleoside analogue for the in vivo imaging of the gene expression of herpes simplex virus type-1 thymidine kinase (HSV1 TK) *Chem Biodivers*. **2006** Mar;3(3):274-83.
- [3] JC Phillips, R Braun, W Wang et al. Scalable molecular dynamics with NAMD. *J Comput Chem*. **2005**, 26, 1781.

Powder diffraction, electron microscopy, focus, charge flipping and zeolites

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As a result of impressive methodological advances in recent years, the determination of a crystal structure from powder diffraction data is no longer a rarity. However, some zeolite structures remain intractable. To address such problems, the powder diffraction data can be supplemented with information from other sources. Both the zeolite-specific structure-solution program *Focus* and the more generally applicable powder charge-flipping (*pCF*) algorithm have been adapted to accommodate such data combinations, and this has allowed the complex structures of TNU-9 (24 Si atoms), IM-5 (24 Si atoms) and SSZ-74 (23 Si atoms) to be solved. The key in all cases was the combination of high-resolution powder diffraction data with information derived from high-resolution transmission electron microscopy (HRTEM) images.

For TNU-9, *Focus* was used to combine the reflection intensities extracted from the powder diffraction pattern with phases and a structure envelope derived from HRTEM images. For the other two, the *pCF* algorithm implemented in *Superflip* [1] was used to effect the combination. Both algorithms work in both direct and reciprocal space, so they are particularly well-suited for bringing data from different sources together, whether the data be in diffraction or real space. Adding even a very limited amount of phase information to the initial (usually random) phases in either algorithm, can make the difference between solving and not solving a structure, and this proved to be the case for TNU-9, IM-5 and SSZ-74.

With 23-24 Si atoms in the asymmetric unit, these are by far the most complex zeolite framework structures known. The approach used to elucidate their structures is not only generally applicable, but many extensions to include other types of data can be envisioned.

[1] Palatinus, L, Chapuis, G (2007) *J. Appl. Cryst.* **40**, 786-790.

Expression and purification of membrane proteins with an emphasis on the hERG channel for the use in biophysical methods

Irina Bauer⁵, Christophe Briand³, Tobias Broger⁵, Brigitte D'Arcy¹, Regine Eibl⁵, David Frasson⁴, Markus Grütter³, Daniel Gyga², Georg Hausammann³, Bernhard Henes⁵, Jana Lamp³, Silvano Landert⁴, Liudmila Polonchuk¹, Martin Sievers⁴, Georg Schmid¹, Bernhard Sonnleitner⁴, Christian Spörri³, Ralf Thoma¹, Tobias Wermelinger⁴ and Michael Hennig¹

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Ion channels represent a class of pharmacologically very interesting protein targets. The modulation of the activity of ion channels by drug molecules has impact on signaling pathways in the human body that can be used for the treatment of diseases. Several years ago, it became evident that several drug molecules inhibit the functionality of the human "ether-a-gogo" potassium channel – hERG causing QT prolongation, also known as "torsades de pointes" – a drug side effect that can not be tolerated. Consequently, several drug molecules were withdrawn from the market and today a systematic assessment of hERG inhibition of drug molecules is performed [1,2]. We use hERG as a model system to investigate and evaluate several routes of heterologous expression of ion channels in different systems like baculovirus (Sf9), *Pichia pastoris*, *Rhodobacter sphaeroides*, HEK293 etc. In addition, several strategies for the use of tags and vector systems are discussed to optimize the level of protein expression as a prerequisite to purify protein in an amount and quality suitable for biophysical methods [3,4]. The project is an excellent example of the close collaboration under the framework of the KTI/CTI ("Science to the market) of industry (Roche) and several academic institutes (organized in the Swiss Biotechnet, NCCR) in order to combine expertise and work forces for a challenging protein.

[1] Sanguinetti, M.C., Mitcheson, J.S. (2005) TIBS **26**, 119-124.

[2] Aronov, A.M. (2005) DDT **10**, 149-155.

[3] Long, S.B., Campbell, E.B., MacKinnon, R., (2006) Science **309**, 897-903.

[4] Kawate, T., Gouaux, E. (2006) Structure **14**, 673-681.

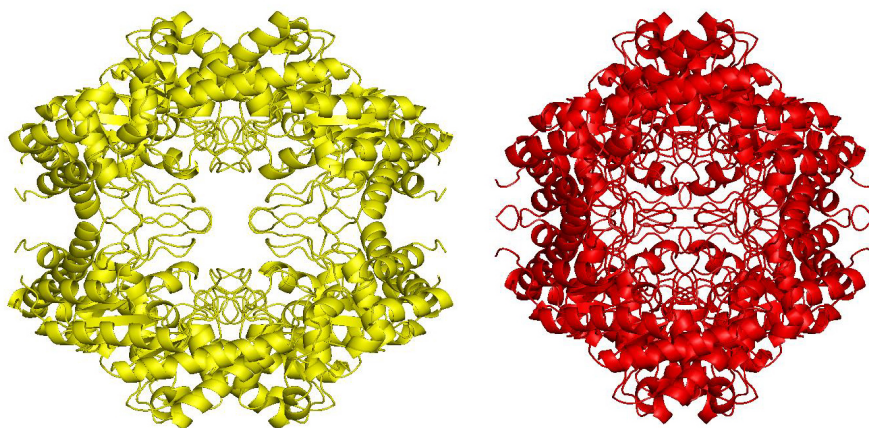
Dehydration-induced phase transition in glucose isomerase

Francesco Gramiccia, Céline Besnard, Yves Pellegrinelli, Sebastian Basso and Marc Schiltz

Laboratoire de Cristallographie, EPFL FSB IPMC, BSP Dorigny, CH-1015 Lausanne, Suisse

Glucose isomerase, which causes the isomerization of glucose to fructose, has a large market in the food industry because of its application in the production of high-fructose corn syrup. In order to fully understand and control the activity of the protein a good knowledge of the structural response of the protein to changes in the environmental conditions is necessary. Since proteins function in aqueous media and nearly half of the volume of protein crystals is occupied by water, protein-water interactions are of great interest.

We have now identified a dehydration-induced phase transition in D-Glucose isomerase from *streptomyces rubiginosus*. The transition, characterized using both powder and single crystal diffraction, occurs at room temperature for relative humidity around eighty percent. After the transition, the crystal totally recovers its crystalline state and diffracting power. The symmetry is reduced from space-group I222 to its subgroup P21212 but the effects of this symmetry break on the structure are subtle. The decrease of the unit-cell volume by more than 15 percent produces more pronounced and interesting structural rearrangements in the crystal (see figure).



In-situ studies of apoferritin crystallization in agarose gel

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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. As a result, understanding the mechanisms of protein crystallization is a major challenge in macromolecular crystallography. Gels such as agarose provide an attractive growth environment for biological crystals. They act by reducing convection in the crystallization environment and trapping the nuclei [1]. We present here an in-situ study of the crystallization of apoferritin in agarose gel in which the crystallization is induced by a front of cadmium salt diffusing along the capillary. The capillary is scanned by a small X-ray beam and low-angle diffraction data are recorded as a function of both the position and the time. By combining the SAXS data with the analysis of the powder diffraction peaks, knowledge can be gained on the mechanism underlying the formation and the growth of the crystallites. We specially discuss the evolution a broad q-peak appearing in the SAXS data before the first Bragg peaks are visible in the powder pattern and its relationship with para-crystalline order appearing in the gel as a prelude to crystallization.

[1] Biertümpfel et al, (2002) Acta Cryst. **D 58** . 1657

Magnetic properties of UMn_2Ge_2 solid solution

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¹Laboratory for Neutron Scattering, ETH Zürich & Paul Scherrer Institut, Switzerland

² Moscow State University, Russia

We have studied crystal and magnetic structure of UMn_2Ge_2 solid solution using neutron diffraction. We have found that below 100K both U and Mn ferromagnetically ordered along c axis whereas over 100K only Mn ions possess magnetic moment. Evolution of magnetic ordering is discussed.

The results compares with our previous studies of $U(Pd/Fe)_2Ge_2$ system [1,2]. Possible mechanism of magnetic properties are discussed

[1] A.M.Balagurov, E.V.Raspopina, V.V.Sikolenko, I.S.Lyubutin, A.S.Stepin, A.V.Griбанov, G.Andre, F.Bouree, H.M.Duh, J.Mag.Mag.Mat. **210**, 225-232 (2000)

[2] V.V.Sikolenko, D.P.Kozlenko, E.V.Pomjakushina, V.Yu.Pomyakushin, A.M.Balagurov, L.Keller, V.P.Glazkov, A.V.Griбанov, I.N.Goncharenko, B.N.Savenko, J. Phys.:Cond.Mat **15**, 2825-2832 (2003)

The crystal structure of $\text{Mg}_2\text{Na}_2\text{NiH}_6$ revisited

Maria Orlova and Klaus Yvon

Laboratory of Crystallography, University of Geneva, Switzerland

The title compound has been reported last year by Kadir and Noréus [1]. It can be classified as a complex metal hydride that contains two sorts of hydrogen atoms, one covalently bonded to nickel by forming tetrahedral NiH_4^{4-} anions, and another more ionic bonded to Mg^{2+} and Na^+ cations only. While the overall structural features appeared to be consistent with those in related hydrides, a study of the bond distances revealed some unusual features such as, for example, rather long metal-metal distances (e.g. $\text{Mg-Ni}=3.67 \text{ \AA}$). Furthermore, a comparison between the observed and calculated X-ray patterns showed significant discrepancies. Thus, we decided to look more closely into this compound by preparing it in accordance with [1]. A hydride sample ($\sim 5\text{g}$ mass) containing $\text{Na}_2\text{Mg}_2\text{NiH}_6$ as a majority phase was studied by using high-resolution powder diffraction on HRPT at SINQ (PSI, Villigen, Switzerland, high intensity mode, $\lambda = 1.8857 \text{ \AA}$, 2θ range $5\text{--}164^\circ$, step size 0.1° , data collection time ~ 16 hours), and its structure was solved ab-initio. Surprisingly, while the space group symmetry of the hydride ($Pnma$) was identical to that reported for the deuteride [1], the atomic coordinates, in particular those of the Mg atoms, and the interatomic distances differed substantially between the hydride and the deuteride (see Fig. 1).

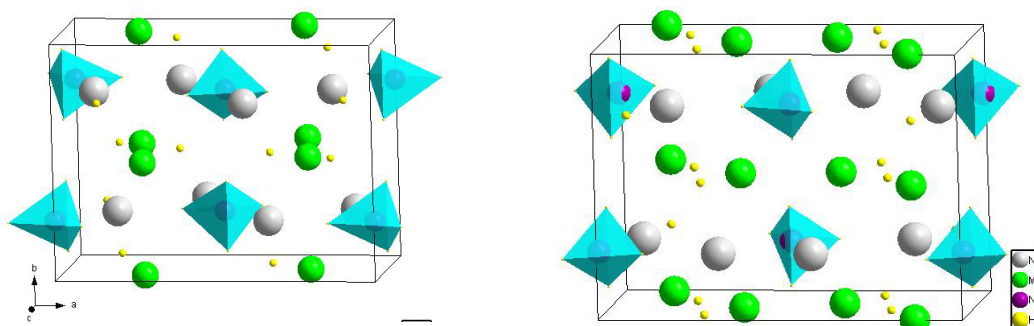


Figure 1. Structure of $\text{Na}_2\text{Mg}_2\text{NiD}_6$ as reported by [1] (left), and of $\text{Na}_2\text{Mg}_2\text{NiH}_6$ [this work] (right).

Clearly, the metal-metal distances of the new model (e.g. $\text{Mg-Ni} = 2.64 \text{ \AA}$) were more in line with those usually observed in complex transition metal hydrides (e.g. Mg_2NiD_4 : $\text{Mg-Ni} = 2.69 \text{ \AA}$), and the calculated X-ray diffraction patterns of the hydride model agreed well with those observed and published. We therefore conclude that the structure model of the hydride is correct, and that the model of the deuteride needs to be revised.

[1] Kadir K., Noréus D. (2007) *Inorg. Chem.* **46**, 2220-2223.

Acknowledgement: We thank Y. Tokaychuk (CNRS, Thiais) for useful discussions and preliminary experiments, and D. Sheptiakov (PSI, Villigen) for help with data collection and analysis.

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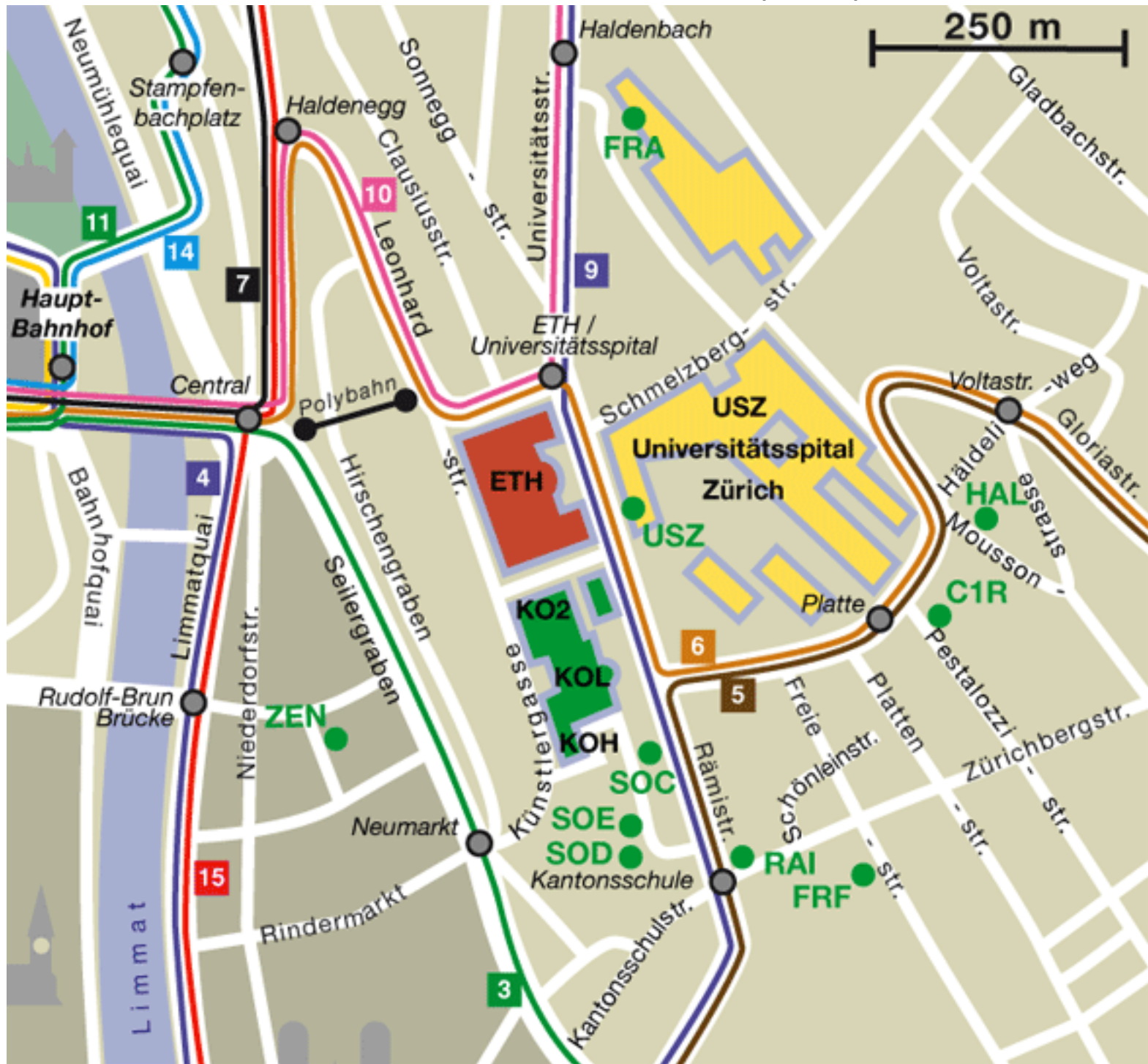
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SINQ: Swiss Spallation Neutron Source All instruments (regular calls)	May 15, Nov. 15	user.web.psi.ch
SμS: Swiss Muon Source All instruments	Dec. 5	user.web.psi.ch
ESRF: European Synchrotron All instruments, long term proposals All instruments, short term proposals	Jan. 15 March 1, Sept. 1	www.esrf.fr www.esrf.fr
SNBL: Swiss Norwegian Beam Line	March 1, Sept. 1	www.esrf.fr/ exp_facilities/BM1A
ILL: Institut Laue Langevin All instruments	Sept. 16, 2008	www.ill.fr
FRM-II All instruments	Jan. 16, July 17, 2009	user.frm2.tum.de

Calendar of forthcoming meetings

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

2008			Abstract Deadline
August 16-22	Zuoz CH	Zuoz 2008, PSI Summer school: Probing the nanometer scale with Neutrons, Photons and Muons	June 30, 2008
August 23-31	Osaka Japan	IUCr-2008, 21 st General Assembly and Congress of IUCr http://www.congre.co.jp/iucr2008	to be announced
August 25-29	Rome Italy	14 th General Conference of the European Physical Society 22 nd General Conference of its Condensed Matter Division http://www.cmdconf.org/eps14/program.html	April 7, 2008
Sept. 9-14	Sydney Australia	WATOC-08 World Association of Theoretical and Computation Chemists, http://www.watoc2008.com/	to be announced
Sept. 8/9	Zürich CH	Annual Meeting 2008 of the SGK/SSCr, joint meeting with the NCCR (Structural Biology) www.structuralbiology.uzh.ch/symposium2008.asp	Aug. 29, 2008
Sept. 9	Zürich	General Assembly/Dinner of the SGK/SSCr	Aug. 2, 2008
Sept. 18-22	Warsaw Poland	EPDIC-11 European Powder Diffraction Conference http://www.epdic-11.eu	April 30, 2008
Sept. 18	Warsaw Poland	Software workshop at EPDIC 11 http://www.sgk-sscr.ch/EPDIC11/SoftwareWorkshop.html	April 30, 2008
Sept. 24-36	Erlangen Germany	Simulationen von Defektstrukturen und Diffuser Streuung, http://www.lks.physik.uni-erlangen.de/diffuse_workshop/indexG.html	
Sept. 29- Oct. 1	Pfäffikon SZ Switzerland	7 th International Workshop on Catalytic Combustion and «Future Concepts in Energy Related Catalysis» 2008 http://iwcc7.web.psi.ch/	expired
Oct. 14-17	Bern CH	Annual Meeting of the Swiss Academy of Science http://www.scnat.ch	to be announced
Nov. 17-20	Ghent Belgium	14 th International Conference on Thin Films http://www.ICTF14.UGent.be	to be announced

2009

Feb. 10-13	Villigen CH	QENS 2009: 9 th International Conference on Quasielastic Neutron Scattering, http://qens2009.web.psi.ch/	Oct. 20, 2008
June 14-20	Castellaneta Italy	ICC14: XIV International Clay Conference http://www.14icc.org/	expired
June 22-24	Kuala Lumpur Malaysia	ICNX 2009: International Conference on Neutron and X-Ray Scattering, http://icsd.ill.fr/ICNX2009.pdf	Jan. 31, 2008
August 14-15	Istanbul Turkey	Symmetry and Crystallography in Turkish Art and Culture, Satellite Conference of the ECM-25 www.lcm3b.uhp-nancy.fr/mathcryst/istanbul2009.htm	to be announced
August 16-21	Istanbul Turkey	ECM-25: European Crystallographic Meeting http://www.ecm25.org	to be announced

2010

to be announced

2011

	Madrid Spain	IUCr-2011, 22 nd General Assembly and Congress of IUCr	to be announced
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2012

Aug. 27-30	Darmstadt Germany	EPDIC-12	to be announced
Aug. 29 – Sept. 3	Darmstadt Germany	ECM-26	to be announced

2013

Aug/Sept.	Bergen Norway	ECM-27	to be announced
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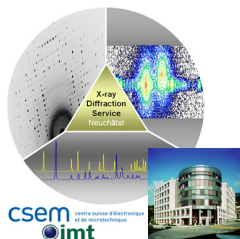
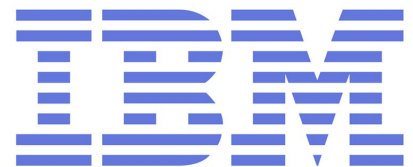
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Membership subsection crystal growth	Yes () No ()
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Major research interests	
Highest degree received	
from university	
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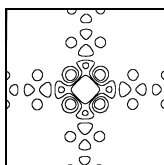
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