

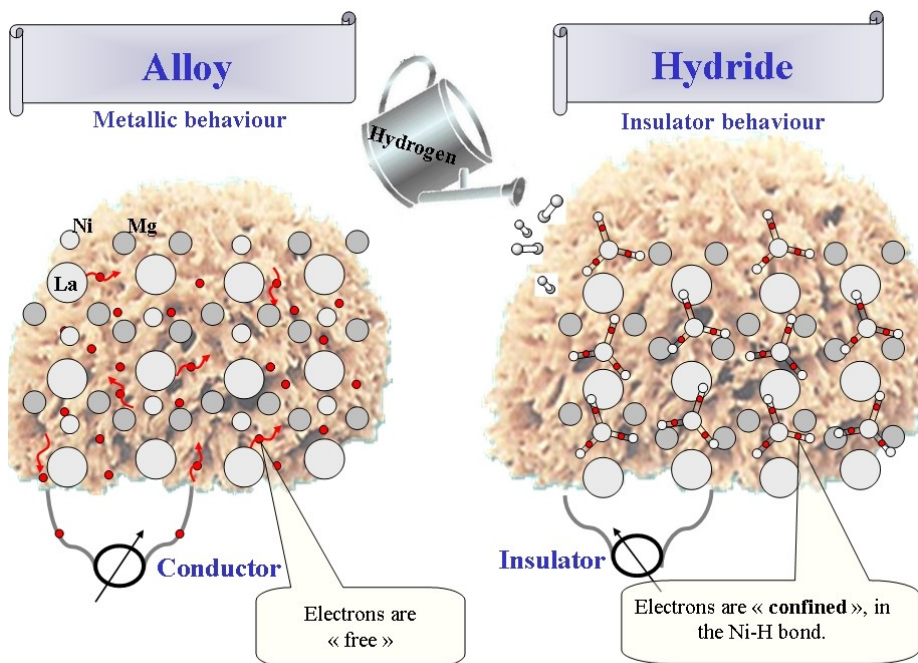


Schweizerische Gesellschaft für Kristallographie  
Société Suisse de Cristallographie

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

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## SGK/SSCr Newsletter No. 66

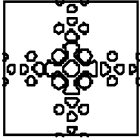
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### Cover page:

Conductor-Insulator transition induced by hydrogenation in a hydrogen "sponge". This transition will be discussed by Jean-Philippe Rapin in a lecture at our Annual Meeting 2005. See his abstract on page 7.



*SGK/SSCr*  
SKT/SCT

*Swiss Society for Crystallography*  
Section for Crystal Growth and Crystal Technology

# **Annual Meeting 2005**

Thursday, October 13

Auditoire 410, Collège propédeutique 2,  
Université de Lausanne, Dorigny

**Lausanne**

*General Theme*

## **Crystallography and Physics**

## Programme

Lecture room : Auditoire 410, Collège propédeutique 2,  
Université de Lausanne, Dorigny, 1015 Lausanne

09h25 – 09h30	<b>Welcome by the President Radovan Cerny, and the local organisers Gervais Chapuis and Marc Schiltz</b>
09h30 – 10h20	Edgar Weckert, DESY, Hamburg « The new radiation sources PETRA III and the European XFEL at DESY »
10h20 – 11h10	Andras Sütő, Hungarian Academy of Science, Budapest « Ab initio structure solution by charge flipping »
11h10 – 11h50	<b>Coffee break / Poster session</b>
11h50 – 12h10	Lukáš Palatinus, EPFL « Charge flipping in superspace »
12h10 – 12h30	Jean-Philippe Rapin, Université de Genève « New examples of a hydrogen-induced metal-semiconductor transition in hydrogen storage materials »
12h30 – 14h00	<b>Lunch / Coffee / Poster session</b>
14h00 – 14h50	Jean-Louis Hodeau, CNRS Grenoble « Resonant diffraction »
14h50 – 15h40	Franz Pfeifer, PSI, Villigen « Coherent x-ray diffraction imaging »
15h40 – 16h00	Selected poster presentation
16h00 – 16h40	<b>Coffee break / Poster session</b>
16h40 – 17h00	Artem R. Oganov, ETHZ « Novel methodologies for predicting crystal structures and phase transition mechanisms »
17h00 – 18h00	<b>General Assembly of the Swiss Society for Crystallography</b>
18h00 – 18h20	<b>Information of the Swiss Steering Committee of the SNBL</b>
From 18h30	<b>Apero followed by Dinner at the Restaurant de Dorigny</b>

**Practical hints to reach Dorigny**

From the Lausanne railway station, you can easily reach the campus by taking the metro to Flon (2 min to the Center of Lausanne) and then the M1 (TSOL) to Dorigny (12 min). Stop at UNIL-Sorge. You can consult a map of the campus at <http://www.unil.ch/central/page2474.html>

The conference building CP2 (no 14 on the map) looks like this  
[http://www.unil.ch/central/page3032\\_fr.html](http://www.unil.ch/central/page3032_fr.html)

**Accommodation**

People requiring accommodation for either the night of Wednesday the 12<sup>th</sup> or Thursday the 13<sup>th</sup> of October can make their own reservation for example on the multi-lingual web site  
<http://www.hotels-and-more.ch/fr/vaud/lausanne/>

**Registration**

The conference dinner will take place on Thursday evening at the Restaurant de Dorigny (building no 12 on the Dorigny map) facing the Savoy Alps. It will cost 40 Sfr, drinks and coffee not included. Students will pay a reduced fee of 30 Sfr. For organisational purposes, please send an email to our secretary, [rossana.papaux@epfl.ch](mailto:rossana.papaux@epfl.ch) until Friday, September 30<sup>th</sup>.

**Poster boards**

Poster can be mounted on wood panels with dimensions 180 (h) x 120 (v), which amount to 2 A0 posters per panel.

**Additional Poster Abstracts**

Posters on any crystallographic subject may be presented during the meeting. Contributors are kindly asked to send their abstracts by e-mail to

[Radovan.Cerny@cryst.unige.ch](mailto:Radovan.Cerny@cryst.unige.ch)

&

[Gervais.Chapuis@epfl.ch](mailto:Gervais.Chapuis@epfl.ch)

The abstracts will be made available under the address

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

# **Lecture Abstracts**

## **Lecture 1**

### **The new radiation sources PETRA III and the European XFEL at DESY**

Edgar Weckert

*HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg, Germany*

At present the main source for synchrotron radiation at DESY is DORIS III, a second generation synchrotron radiation source with 10 wiggler and about 30 bending magnet beamlines. Being a second generation source operating at 4.5 GeV particle energy, DORIS III still is a powerful light source for the investigation of large samples with high-energy X-rays. For this reason a new beamline for materials science, texture and strain analysis, and microtomography is being constructed by the GKSS research center at DORIS III. At the same beamline also a high pressure station for larger samples will be installed by the GFZ research center.

However, due to the large photon beams at DORIS III, all applications needing an extremely small beam focus, high photon beam brilliance or coherent X-rays can hardly be carried out. For that reason DESY has decided to reconstruct its 2.3 km long PETRA II storage ring into a third generation synchrotron radiation source called PETRA III from mid 2007 on. A technical design report about this project has been published in spring 2004 [1]. PETRA III will be operated at a particle energy of 6 GeV and its emittance will be 1 nmrad, which is a world record low value for a high energy storage ring. Due to these parameters PETRA III will be the most brilliant storage ring based X-ray source, enabling a wealth of new experimental techniques like sub 100 nm focusing or experiments exploiting coherent photons. Planning and R&D for PETRA III is in an advanced stage and the first components for the new storage ring sections have already been ordered. The scientific program of the phase I beamlines has been decided and detailed planning in discussion with the user community is ongoing.

Probably even more exciting than the most brilliant synchrotron radiation storage ring PETRA III are DESY's free electron laser (FEL) activities. In spring 2005 the VUV-FEL facility achieved first lasing at 30 nm wavelength and has become

operational for users. The envisaged smallest wavelength at this facility will be 60 Å in its final stage. The measured pulse length has been 20 fs. A FEL provides in a single 100 fs long pulse almost the same number of photons as a third-generation storage ring in one second, which is  $10^8$ - $10^{10}$  times more in peak brilliance compared to present day state of the art storage rings. These short pulses are extremely well suited for all kinds of time-resolved studies at ultra-short time scales.

DESY's main future project, however, is to take the lead in the construction of the European X-ray free electron laser (XFEL). This laser will provide 100 fs long X-ray pulses with wavelengths below 1 Å and more than  $10^{12}$  photons per pulse. The radiation of the XFEL will allow investigating matter at the fs time scale and at atomic length scales simultaneously. Therefore, the XFEL will be the ideal tool for probing the dynamic properties of matter at extremely high resolution. These FEL sources provide, in addition, beams that are transversely coherent, enabling e.g. diffraction also from non translation-periodic objects and allowing for totally new imaging techniques.

The talk will give an overview about the scientific possibilities at the different sources and report on the status of these projects.

[1] [http://www-hasyllab.desy.de/facility/upgrade/petra\\_tdr.htm](http://www-hasyllab.desy.de/facility/upgrade/petra_tdr.htm)

## **Lecture 2**

### **Ab initio structure solution by charge flipping**

András Sütő

*Research Institute for Solid State Physics, Hungarian Academy of Sciences*

In a joint work with Gábor Oszlányi, published recently [1], we proposed a simple *ab initio* Fourier recycling method for structure solution, based on high resolution X-ray diffraction data. In the original version, in real space the sign of the charge density below a (positive) threshold is changed; in reciprocal space the unweighted  $F_{\text{obs}}$  map is applied. The iteration is unconditional, the  $R$  factor is used only for monitoring the convergence. While this algorithm works fairly well on synthetic data for a wide range of structures, a considerable improvement could be obtained with a new version, which complements the phase exploration in reciprocal space. Instead of prescribing observed moduli of all structure factors, weak reflections are treated separately: their calculated moduli are accepted unchanged and their calculated phases are shifted by a constant  $\Delta\varphi = \pi / 2$ . This means that the observed data of weak reflections are *not used* in the

iteration, except for the knowledge that they are indeed weak. The improvement is drastic, in some cases the success rate is increased by a factor of 10, in other cases a previously unsolvable structure becomes solvable. Early applications can be found in papers [2-4].

- [1] G. Oszlányi & A. Sütő, *Acta Cryst.* **A60**, 134-141 (2004); *ibid.* **A61**, 147-152 (2005).
- [2] J. S. Wu, J. C. H. Spence, M. O'Keeffe & T. L. Groy, *Acta Cryst.* **A60**, 326-330 (2004).
- [3] L. Palatinus, *Acta Cryst.* **A60**, 604-610 (2004).
- [4] J. S. Wu & J. C. H. Spence, *Acta Cryst.* **A61**, 194-200 (2005).

## Lecture 3

### Charge Flipping in Superspace

Lukáš Palatinus

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“Charge flipping” is an algorithm for *ab initio* structure solution from X-ray diffraction data that is based on alternating modifications of a trial electron density in direct and reciprocal space [1]. This algorithm makes no use of the atomicity of the chemical structure. Instead it is based on the observation that the electron density of a crystal consists of a small number of high-density areas separated by large areas with very small electron density. This property is common to both electron densities of periodic structures and superspace electron densities of modulated structures. Therefore, charge flipping can be generalized towards superspace and used to reconstruct the superspace electron densities [2]. Up to now the structure solution of incommensurately modulated structures has been a two-step procedure involving solution of the basic periodic structure followed by the determination of the modulation. Charge flipping offers for the first time the possibility to solve the modulated structures directly in superspace, avoiding the often tedious task to construct and refine the basic structure. Charge flipping was successfully applied to solve several modulated crystal structures including several organic and organometallic compounds with complex modulations [2].

- [1] Oszlányi G., Sütő A., *Acta Cryst.*, 2004, **A60**, 134.
- [2] Palatinus L., *Acta Cryst.*, 2004, **A60**, 604.

## Lecture 4

### **New examples of a hydrogen-induced metal-semiconductor transition in hydrogen storage materials**

Jean-Philippe Rapin

*Laboratoire de Cristallographie, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève 4*

Solid-state metal hydrides provide a safe and efficient way of storing and transporting hydrogen. As a result of recent work [1] novel intermetallic compounds based on lanthanum, magnesium and nickel/palladium have been discovered (called “alloys” thereon). They absorb reversibly hydrogen near ambient conditions thus forming stoichiometric and ordered hydrides that exhibit remarkable electrical properties. The structures were solved ab-initio by neutron and synchrotron powder diffraction. The hydrogen free alloys crystallise with a centrosymmetric, orthorhombic structure (*Cmcm*). Hydrogenation reduces the symmetry to non-centrosymmetric  $P2_12_12_1$  for the palladium compound and to monoclinic for the nickel compound ( $P2_1/c$ ). Electrical properties were studied by a combination of experimental and theoretical work. They reveal metallic behaviour for the alloy and non-metallic behaviour for the hydride. The “confinement” of “free” electrons in the alloy into Ni-H or Pd-H bonds in the hydride is represented in a schematic manner in the figure on the title page.

[1] K. Yvon, G. Renaudin, C.M. Wei and M.Y. Chou, *Physical Review Letters*, **94** (2005), 066403.

## Lecture 5

### **Resonant Diffraction**

Herve Palancher, Elena Nazarenko, Emilio Lorenzo, Yves Joly,  
Eric Dooryhee, Jean-François Berar, Jean-Louis Hodeau

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*Resonant Diffraction* refers to the modification of scattering intensity due to absorption processes involving interactions between the X-ray beam and the atoms in the sample. This interaction contains the chemical and *short-range order* sensitivity of absorption as well as the *long-range order* sensitivity of diffraction. This enables resonant diffraction to be exploited to perform (i) site selective spectroscopy to extract information on site symmetry, distortion, orbital or charge ordering, and (ii) element selective diffraction experiments.

Full spectra obtained by Diffraction Anomalous Near Edge Spectroscopy experiments (DANES) give information on the local symmetry and/or the valence state of the resonant atom with the same sensitivity as for X-ray Absorption Near Edge Spectroscopy experiments (XANES) but with the additional *site selectivity*. Using polarized X-rays, DANES spectra can depend on the orientation of the local chemical environment of the resonant scatterer with respect to the beam polarization direction. The anomalous scattering factor must be replaced by a *tensor* to take polarization of both incident and diffracted beams into account.

The *chemical sensitivity* of resonant (or anomalous) diffraction allows contrast studies of a selected atom in a given crystallographic site. This has been demonstrated a long time ago but is not largely used. However, we show that, even in powder samples with considerable reflection overlap and with a basically known framework, the use of “*dispersive difference*” electron density maps allows an easy localisation of resonant atoms. On the other hand, the use of “*anomalous difference patterns*” enables good agreement factors to be achieved for accurate localisation and validates the resonant scattering method for *contrast studies* in complex powders with mixed occupancy sites.

After a review on different possibilities of resonant diffraction, we will focus on experimental strategies and specific requirements needed to fully extract the rich but tiny resonant information. Our presentation will deal with multilayers, single crystals and powders of inorganic oxides, including perovskite, magnetite<sup>[1]</sup> and zeolite<sup>[2]</sup>.

[1] E. Nazarenko, J. E. Lorenzo, Y. Joly, J-L. Hodeau, D. Mannix & C. Marin  
Direct experimental evidence of charge ordering in the low temperature phase of magnetite, submitted.

[2] H. Palancher, J-L. Hodeau, C. Pichon, J.F. Bézar, J. Lynch, B. Rebours & J. Rodriguez-Carvajal  
Direct localization of atoms in mixed occupancy powders by resonant contrast diffraction  
Angew. Chem. Int. Ed., (2005), **44**, 11, 1725.

## Lecture 6

### Coherent x-ray diffraction imaging of single crystalline nanocubes

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*b) Department of Chemistry, University of Washington, Seattle, WA 98195-1700, USA.*

*c) Department of Physics, University of Illinois, Urbana, Illinois, 61801, USA.*

X-ray crystallography has been proven to be an extremely efficient investigation method to solve the structure of matter at the atomic scale. Although several methods have been employed to circumvent the intrinsic phase problem, other limitations do exist for classical x-ray crystallographic methods. As has recently been shown, a combination of coherent x-ray diffraction together with a computer based phase retrieval method can be used to overcome these limitations [1,2,3].

In this context, we have studied the feasibility of pushing the limits of imaging small crystals by using coherent x-ray diffraction into the nanometer range. For this purpose we have used chemically synthesized, single crystalline silver nanocubes with an average typical size of 175 nm [4]. The coherent diffraction pattern has been measured using monochromatic x-rays with an energy of 8.5 keV and successfully been inverted into real space images.

Furthermore, we have investigated the possibility of using focusing optics (i.e. Fresnel Zone Plates and Kirk Patrick-Baez mirrors) for coherent x-ray diffraction experiments [5]. In order to precisely characterize their effect on the coherence properties of the beam we have developed an interferometric method to measure the full coherence function of a hard x-ray beam [6].

#### References:

- [1] D. SAYRE, *Imaging Processes and Coherence in Physics*, Springer Lecture Notes in Physics, Vol. **112**, 229 (1980).
- [2] J. MIAO, P. CHARALAMBOUS, J. KIRZ, and D. SAYRE, *Extending the methodology of X-ray crystallography to allow imaging of micrometer-sized non-crystalline specimens*, *Nature* **400**, 342 (1999).
- [3] G.J. WILLIAMS, M.A. PFEIFER, I.A. VARTANYANTS, and I.K. ROBINSON, *Three-dimensional Imaging of Microstructure in Gold Nanocrystals*, *Phys. Rev. Lett.* **90**, 17 (2003).
- [4] YUGANG SUN and YOUNAN XIA, *Shape-Controlled Synthesis of Gold and Silver Nanoparticles*, *Science* **298**, 2176 (2002).
- [5] I.K. ROBINSON, F. PFEIFFER, I.A. VARTANYANTS, Y. SUN, and Y. XIA, *Enhancement of coherent X-ray diffraction from nanocrystals by introduction of X-ray optics*, *Optics Express* **11**, 2329 (2003).
- [6] F. PFEIFFER, O. BUNK, T. WEITKAMP, C. DAVID, J.F. VAN DER VEEN, AND I.K. ROBINSON, *Shearing Interferometer for quantifying the coherence of hard x-ray beams*, *Phys. Rev. Lett.* **94**, 164801 (2005).

## Lecture 7

### **Advances in theoretical crystallography: novel methodologies for predicting crystal structures and phase transition mechanisms.**

Artem R. Oganov

*Laboratory of Crystallography, Department of Materials, ETH Hönggerberg,  
HCI G 515, Wolfgang-Pauli-Str. 10, CH-8093 Zurich, Switzerland*

Crystal structure prediction (i.e. finding the stable structure for a given compound at given P-T conditions) is one of the most fundamental and most difficult problems to solve. In spite of numerous attempts, there has been no general and efficient solution to this problem. Finding a way to solve this problem would greatly expand the power of computer simulations because:

1. It would allow design of new materials and their properties entirely on the computer.
2. It would open up ways to rapidly discover new (often unusual) structures at high pressures and temperatures, where direct experimentation is very difficult or impossible. This would greatly improve our understanding of planetary interiors and of chemical bonding in materials at extreme conditions [1-3].
3. It would help to solve many disordered, defective or large structures, where purely experimental approach may be insufficient.

Our efforts in this direction have culminated in the formulation of the USPEX (Universal Structure Predictor: Evolutionary Crystallography) method and the corresponding computer simulation code (Glass, Oganov, Hansen, in prep.; Oganov & Glass, in prep.) based on our evolutionary algorithm coupled with quantum-mechanical total energy calculations. This methodology has been applied to a wide range of materials (e.g., H<sub>2</sub>, C, Si, N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, Cl<sub>2</sub>, Xe, Fe, WB<sub>3</sub>, MgCO<sub>3</sub>, CaCO<sub>3</sub>, MgSiO<sub>3</sub>, Al<sub>2</sub>O<sub>3</sub>, NO<sub>2</sub>, etc.) including ionic, covalent, metallic, and molecular crystals, especially at high pressure. It proved to be vastly superior to other computational methods in terms of efficiency and reliability. Our method always found the correct most stable structure when experimental data were available. For experimentally less-well studied cases, we have been able to solve the previously unsolved high-pressure structures (O<sub>2</sub>, MgCO<sub>3</sub>, CaCO<sub>3</sub>, NO<sub>2</sub>), clarify situations controversial from the experimental point of view (N<sub>2</sub>, Fe, Al<sub>2</sub>O<sub>3</sub>), and predicted entirely new and unexpected structures (H<sub>2</sub>, F<sub>2</sub>). These show new, hitherto unexpected aspects of chemical bonding of solids at extreme conditions.

To study phase transformation mechanisms, we employ a different method, metadynamics [4]. We have found that metadynamics is capable of predicting also the mechanism of plastic deformation of solids. This has been exploited in order to clarify the rheological behaviour of the Earth's lowermost mantle [5].

[1] Oganov A.R., Ono S., 2004, *Nature* **430**, 445-448.

[2] Oganov A.R., Ono S., 2005, *Proc. Natl. Acad. Sci.* **102**, 10828-10831.

[3] Oganov A.R. et al., 2005, *Phys. Rev. B* **71**, 064104.

[4] Martonak R., Laio A., Parrinello M., 2003, *Phys. Rev. Lett.* **90**, 075503.

[5] Oganov et al., Submitted to *Nature*, 2005.

## **Poster Abstracts**

### **Atomic Displacement Parameters and Specific Heat of *p*-Dichlorobenzene Polymorphs between 10 and 230 K**

Thammarat Aree<sup>a</sup>, Marc Hostettler<sup>a</sup>, Karl W. Törnroos<sup>b</sup>,  
Dmitry Chernyshov<sup>a,c</sup>, Hans-Beat Bürgi<sup>a</sup>

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<sup>c</sup>*Petersburg Nuclear Physics Institute, Russia*

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Synchrotron data for the  $\alpha$ - and  $\beta$ -polymorphs of *p*-dichlorobenzene (*p*-DCB) between 10 and 230 K were collected to 0.5 Å resolution at the ESRF and refined with a multipole model in order to deconvolute thermal motion from valence bonding density. Sealed tube data of the  $\gamma$ -polymorph were collected between 100 and 180 K to 0.7 Å resolution and refined with a spherical atom model. The multi-temperature atomic displacement parameters (ADPs) were analyzed in terms of libration and translation frequencies [1]. From the six external vibration frequencies and the intramolecular vibration frequencies from high-level DFT calculations heat capacities  $C_v$  were calculated with molecular Einstein and Debye models and found to be in fair agreement with  $C_p$  from calorimetric measurements [2].

[1] Bürgi H.-B., Capelli S.C., Birkedal H., *Acta Cryst.* 2000, **A56**, 425.

[2] Dworkin A., Figuière P., Ghelfenstein M., Szwarc H., *J. Chem. Thermodyn.* 1976, **8**, 835.

### **Polymorphism and Photochromism of Salicylideneaniline**

Frédéric Arod,<sup>a</sup> Manuel Gardon,<sup>a</sup> Philip Pattison,<sup>a,b</sup> Kurt Schenk<sup>a</sup>, and Gervais Chapis<sup>a</sup>

<sup>a</sup>*Laboratoire de Cristallographie, École Polytechnique Fédérale de Lausanne, Switzerland*

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Organic compounds exhibiting photo- or thermochromicity are of considerable interest owing to their properties and possible applications. The photochromism of salicylideneaniline (SA) was discovered by Senier *et al.* at the beginning of last century, and in 1964, Cohen *et al.* [1] observed its polymorphism.

It is generally accepted that the stable form of SA in the ground state is the enol form, with an intramolecular hydrogen bond between the hydroxyl proton and the nitrogen atom. Upon photoexcitation of this enol form with UV light, it undergoes an ultrafast proton transfer from the hydroxyl group to the nitrogen, due to the electronic redistribution in the excited state. The proton transfer generates a keto tautomer in the excited state.

We report on the alpha-2-polymorph structure of SA in the ground state [2]. We also describe a new polymorph, beta, which features a planar SA molecule and is therefore thermochromic.

We did also revisit the alpha-1-polymorph structure of SA described by Destro *et al.* [3], but reconsidering their hypothesis. We suggest a lowering of the symmetry with the aim to improve the structure.

[1] Cohen, M.D.; Schmidt, G.M.J.; Flavian, S. *J. Chem. Soc.* **1964**, 2041-2051.

[2] Arod, F.; Gardon, M.; Pattison, P. & Chapuis, G. *Acta Cryst.* **2005**, C61, o317-o320.

[3] Destro, R.; Gavezzotti, A. & Simonetta, M. *Acta Cryst.* **1978**, B34, 2867-2869.

## Is your Crystal representative of the Bulk?

G. Bernardinelli and H. D. Flack

*Laboratoire de Cristallographie, Université de Genève*

Structure analysis by X-ray diffraction is commonly carried out on just **one** single crystal. The physical, chemical, pharmaceutical, biological and structural properties of this one crystal can only be characteristic of the bulk under certain circumstances. In particular for bulk samples which are mixtures, or whose purity is questionable, an excellent ploy is to characterize the one single crystal used for the diffraction experiment. However until recently a difficulty has been its small mass *ca.* 1 µg. Thermochemical characterization by way of differential scanning calorimetry (DSC) can provide clear evidence on purity, phase transitions and solid-solution formation. For enantiomeric mixtures both circular dichroism (CD) and enantioselective chromatography, but not optical activity, may be applied to such a single crystal taken into solution.

As a first case study, a determination of absolute configuration was achieved from X-ray diffraction and CD measurements on crystals obtained from a racemate in the bulk by spontaneous resolution to give a tricky racemic

conglomerate. Crystals were either enantiopure but twinned by a pure rotation, or twinned by inversion in various proportions. In the second case study of an absolute-configuration determination from an enantiopure sample, the optical activity and CD spectrum were far too weak to be useful to characterize the enantiomer. However enantioselective chromatography on the single crystal taken into solution provided the necessary characterization.

## How close can Halogen Atoms get in a Crystal Triphenylmethylbromide

Céline Besnard<sup>1</sup>, Fabrice Camus<sup>1</sup>, Mogens Christensen<sup>2</sup>,  
Marc Fleurant<sup>1</sup>, Andy Fitch<sup>3</sup>, Phil Pattison<sup>1,4</sup>, Marc Schiltz<sup>1</sup>

<sup>1</sup>Laboratory of Crystallography, EPFL, Lausanne, Switzerland

<sup>2</sup>University of Aarhus, Denmark

<sup>3</sup>ESRF Grenoble, France

<sup>4</sup>Swiss-Norwegian BeamLine, ESRF, Grenoble, France

The crystal structure of triphenylmethylbromide (TPMBr) displays unusually close halogen...halogen contacts between neighbouring molecules. The shortest Br...Br distance is 3.203 Å at room temperature, which is about 0.5 Å smaller than the sum of the van-der-Waals radii [1]. An investigation of the crystal structure of TPMBr as a function of temperature was performed, to check if the lattice contraction would allow a further compression of the Br...Br contacts.

We found that a reversible phase transition occurs at about 160K, where the single crystal splits up into different domains. The so-formed twinned crystal recovers back to a single domain on passing through the phase transition back to the high temperature form. Analysis of the twinned data allowed us to solve the structure of the low temperature phase, which turns out to be isomorphic to one of the three known polymorphs of triphenylmethylchlorid (TPMCl) [2]. Inspection of the low and high temperature structures reveals the mechanism of the phase transition: upon lowering the temperature, the Br...Br distances decrease down to a limiting value at 160K. Beyond that point, the molecules undergo a rearrangement whereby the C-Br bonds are tilted away from the 3 fold-axis, thus leading to a lowering of the crystal symmetry from P-3 to P-1. We observed the same transition to occur for TPMCl, but at a higher temperature (260K).

[1] Dunand A., Gerdil R., *Acta Cryst.*, 1984, **B40**, 59.

[2] Kahr B., Carter R.L., *Mol. Cryst. Liq. Cryst.*, 1992, **219**, 79.

## **X-ray induced changes in organic and biological crystalline materials**

F. Camus<sup>a</sup>, C. Besnard<sup>a</sup>, M. Fleurant<sup>a</sup>, I. Margiolaki<sup>b</sup>, P. Pattison<sup>a,c</sup>, M. Schiltz<sup>a</sup>

<sup>a</sup>*Laboratory of Crystallography, EPFL, Switzerland*

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<sup>c</sup>*Swiss-Norwegian Beamlines, ESRF, Grenoble, France*

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The investigation of radiation-induced processes in organic and biological molecules is of importance for gaining a better understanding of the fundamental mechanisms by which certain compounds (e.g. halogenated nucleotides) induce a radio-sensitizing action and can thus be used to improve anticancer radiotherapies. The study of radiation-induced processes in macromolecules is also of considerable interest in the fields of structural biology and genomics, since current progress in synchrotron protein crystallography is hampered by radiation damage in the samples.

We have carried out powder diffraction measurements to investigate structural changes as a function of X-ray irradiation in organic and biological crystals. In these experiments, synchrotron radiation is used both to irradiate the samples and collect diffraction data. Powder diffraction is employed to monitor radiation-induced changes in the unit cell and microstructural parameters (crystallite size and lattice strain) in crystals of native and halogenated nucleobases as well as in other small-molecule model compounds. Similar experiments were carried out also on macromolecular crystals. Our aim in these studies is to investigate radiation-induced changes as a function of temperature, wavelength and X-ray dose rate. Attempts to interpret the observed unit-cell expansions in terms of radiation-induced structural modifications in the crystal will be discussed.

**FOX: a friendly tool to solve crystal structures from powder diffraction**Radovan Černý<sup>I</sup> and Vincent Favre-Nicolin<sup>II</sup><sup>I</sup> *Laboratoire de Cristallographie, Université de Genève, 24, quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland*<sup>II</sup> *Université Joseph Fourier and CEA, DRFMC/SP2M/NRS, 17, rue des Martyrs, F-38054 Grenoble Cedex 9, France*

Structural characterization from powder diffraction by direct space methods has been largely improved in the last 15 years. The success of the method very much depends on a proper modeling of the structure from building blocks. The modeling from larger building blocks improves the convergence of the global optimization algorithm by a factor of up to ten. However, care must be taken about the correctness of the building block like its rigidity, deformation, bonding distances and ligand identity. Dynamical Occupancy Correction implemented in the direct space program FOX [1,2] has proved to be useful when merging excess atoms, and even larger building blocks like coordination polyhedra. It allows also joining smaller blocks into larger ones in the case when the connectivity was not *a priori* evident from the structural model. The effect of modeling by correct structural units will be shown on several examples of non-molecular and molecular structures.

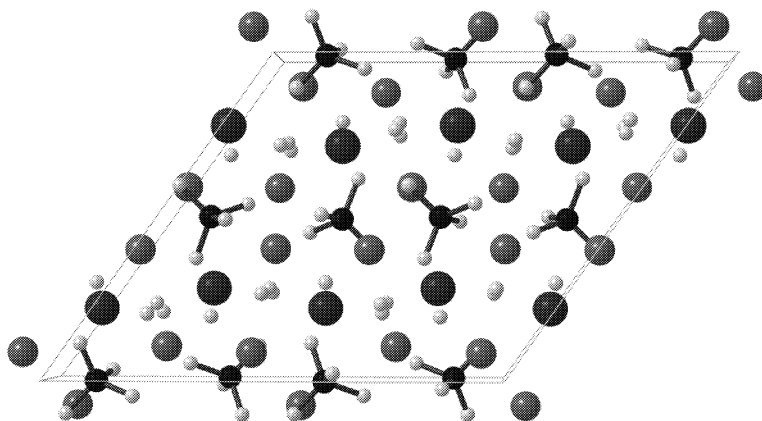


Figure: Monoclinic structure ( $P2_1/c$ ) of  $\text{LaMg}_2\text{NiD}_7$  [3] modeled by two  $[\text{NiD}_4]$  tetrahedra, two La, four Mg and six D atoms.

- [1] Favre-Nicolin, V., and Černý, R. (2002). "FOX, "Free Objects for Crystallography": a modular approach to *ab initio* structure determination from powder diffraction," *J. Appl. Cryst.*, **35**, 734-743.
- [2] Favre-Nicolin, V., and Černý, R. (2004). "A better FOX: using flexible modeling and maximum likelihood to improve direct-space *ab initio* structure determination from powder diffraction", *Z. Kristallogr.*, **219**, 847-856.
- [3] Renaudin, G., Guénée, L., and Yvon, K. (2003). "LaMg<sub>2</sub>NiH<sub>7</sub>, a novel quaternary metal hydride containing tetrahedral [NiH<sub>4</sub>]<sup>+</sup> complexes and hydride anions," *J. Alloys Compounds*, **350**, 145-150.

## **Centrosymmetric structures refined as non-centrosymmetric: a study of the Flack parameter**

H. D. Flack and G. Bernardinelli

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A very recent study by Clemente of structures published in *Inorganica Chimica Acta* provides an extensive set of centrosymmetric crystal structures refined as being non-centrosymmetric. We have examined these “wrong” structures to understand the behaviour of the Flack parameter for a centrosymmetric structure refined as non-centrosymmetric. Many have origin-free directions in the non-centrosymmetric description. Frequently insufficient data have been measured. Values obtained for the Flack parameter have been analyzed. With sufficient data coverage, a value close to 0.5 is obtained. With insufficient data, a value near to zero has been observed and explained. The inverted structure would also lead to a value of zero for the Flack parameter. Many of these structures qualify for the *ORTEP-of-the-Year* prize.

## **Radiation-induced debromination in nucleic acids monitored by polarized X-ray absorption spectroscopy on single crystals**

Marc Fleurant<sup>1</sup>, Fabrice Camus<sup>1</sup>, Céline Besnard<sup>1</sup>, Eric Ennifar<sup>2</sup>,  
Philippe Dumas<sup>2</sup>, Phil Pattison<sup>1,3</sup>, Marc Schiltz<sup>1</sup>

<sup>1</sup>*Laboratoire de Cristallographie, EPFL, Lausanne*

<sup>2</sup>*Institut de Biologie Moléculaire et Cellulaire, CNRS Strasbourg*

<sup>3</sup>*Swiss-Norwegian Beamlines (SNBL) at the ESRF, Grenoble*

The application of radiosensitizing halogenated nucleotides for therapeutic cancer treatments using synchrotron X-rays is currently under investigation. It is believed that the primary radiation-induced reaction is a dehalogenation, leading to highly reactive radical species. In a different light, halogenated nucleic acids have also been used in macromolecular crystallography to solve the structure of nucleic acids by anomalous scattering techniques. However, for brominated compounds, a relative moderate X-ray dose can induce sufficient debromination to prevent structure determination.

In the present study, we show that polarized absorption spectra on single crystals can yield useful information about radiation-induced reactions. Polarization effects in X-ray absorption spectra recorded on oriented single crystals enable an enhanced detection of features occurring in certain crystal and/or molecular directions. We present here time-resolved polarized X-ray absorption measurements taken on a single crystal of a brominated 23-nucleotide RNA fragment corresponding to the dimerization-initiation site (DIS) of HIV-1(Lai) genomic RNA. The radiation-induced dissociation of the bromine atom from the nucleotide is concomitant with a change in symmetry of the immediate chemical environment of the Br atoms (from highly anisotropic to spherically symmetric). This symmetry change manifests itself as a change of linear X-ray dichroism near the Br *K*-edge.

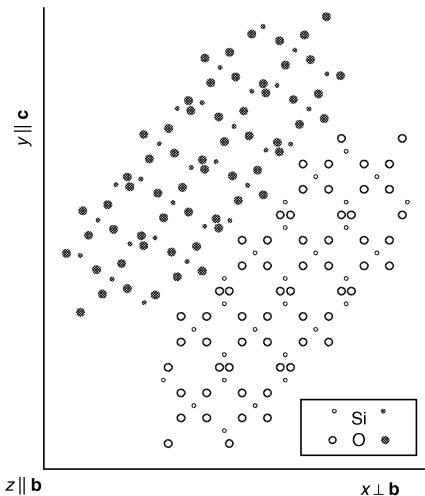
These measurements show that the nature and the progress of the radiation-induced debromination reaction can be followed easily by absorption or fluorescence measurements, especially if the polarization direction is nearly parallel to the C–Br bonds. Since this type of spectra can be easily and quickly recorded, polarized X-ray absorption emerges as a useful tool for studying radiation-induced reactions in the solid state and for monitoring radiation damage in macromolecular crystallography.

## Quartz Aggregates Revisited

Hans Grimmer

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Condensed Matter Research with Neutrons and Muons, Paul Scherrer Institut,  
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Quartz aggregates formed by coalescence of macroscopic quartz crystals in the magma or in hydrothermal solution are considered. If the individuals have  $\{1\ 0\ -1\ 1\}$  faces in contact, there will be two special cases: parallel intergrowths and intergrowths that agree in orientation and contact plane with Esterel twins grown from a twinned nucleus.



*Model of an Esterel twin boundary in  $\beta$ -quartz. The two crystallites are related by a mirror reflection  $\parallel (1\ 0\ -1\ 1)$  followed by a translation in the reflection plane.*

For all other known cases, i.e. when the relative orientation satisfies the Japan, Sardinian, Tiflis, Zyndel-A or Samshvildo law, both individuals have exactly coinciding short symmetry translations in only one direction in the contact plane (monoperiodic twins). If a rhombohedral face is in contact with a prism face, monoperiodic twins will occur if the relative orientation satisfies the Zinnwald, Disentis or a proposed hypothetical law. The orientation of the two lattices can be expressed by a  $180^\circ$  rotation about an axis with low indices independent of  $c/a$  in case of the Esterel, Japan and Sardinian law. The same is true for the Tiflis and Zyndel-A laws only if they are redefined, and not at all in case of the Samshvildo, Zinnwald, Disentis and hypothetical law. When the two individuals have rhombohedral faces in contact, there will even be exact 2-dimensional coincidence (multiplicity  $\sigma$ ) in the contact plane and exact 3-dimensional coincidence (multiplicity  $\Sigma$ ) in space if the square of the axial ratio  $c/a$  is rational. Indications are found that (despite their high values) these multiplicities may be related to the frequency of occurrence of intergrowths in low- and high-quartz.

## The organic modulated structure of 3,4-diphenyl-2a,5a,6,7,8,8a,8b-heptahydro-furo[4,3,2-de]chromen-2-one

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Antonia Neels<sup>c</sup>, Kurt Schenk<sup>a</sup>, Gervais Chapuis<sup>a</sup>

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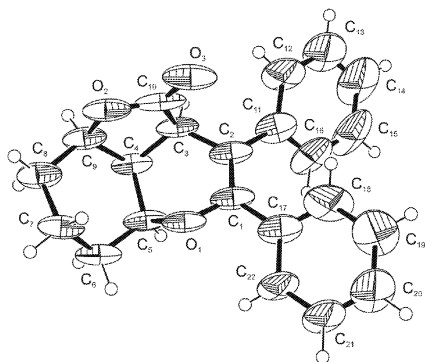
<sup>c</sup> *Institut de Chimie, Université de Neuchâtel, Av. de Bellevaux 51, Case postale 2, CH-2007 Neuchâtel, Switzerland*

The incommensurate structure of the title compound, with formula  $C_{22}H_{20}O_3$ , is presented. Data collection was performed on a single crystal, at 173 K, on a Stoe II image plate diffractometer. The average structure is monoclinic, space group  $P2_1/c$ , with cell parameters  $a = 7.2526(9) \text{ \AA}$ ,  $b = 24.952(3) \text{ \AA}$ ,  $c = 9.896(1) \text{ \AA}$ ,  $\beta = 106.646(8)^\circ$ .

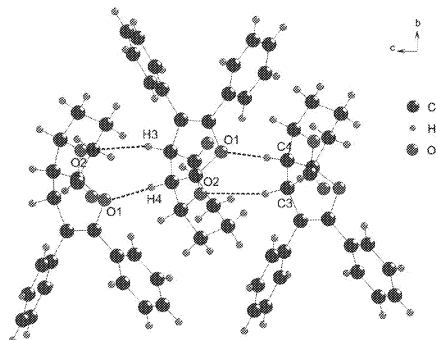
The refinement was performed using some constraints in hydrogen atomic positions, taking into account geometrical considerations. Atomic displacement parameters (ADP) were also restrained with isotropic ones fixed to 1.2 times the equivalent ADP of the neighbour C atom. We used the program JANA2000 (Petříček, 2003) to refine the average and the modulated structure.

The average structure was found with huge ADP values (Fig. 1), which were considerably reduced by introducing a displacive modulation wave function, taking into account satellite reflections visible up to second order on reciprocal space reconstructions. All ADP values became quasi-isotropic, and the main displacement of the molecule occurs along the long axis of the structure.

The study of atomic distances reveals three intermolecular C-H $\cdots$ O hydrogen bonds, two of them linking together the non-phenyl part of the molecule (Fig. 2), and the last one linking this part to a phenyl ring of another molecule.



**Fig. 1:** The molecular structure, corresponding to the average structure, showing 50% probability displacement ellipsoids and the crystallographic numbering scheme. H atoms are drawn as open circles for clarity.



**Fig. 2:** Representation of the packing of the structure showing two of the hydrogen bonds linking the non-phenyl part of the molecules.

### Reference:

Petríček, V., Dušek, M., Palatinus, L. JANA2000. The crystallographic computing system (2003) Institute of Physics, Praha, Czech Republic.

## Ab initio simulations on the W-phase of the Al-Co-Ni system

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Switzerland*

The W-phase [1] is the highest stable approximant of the decagonal quasicrystal known in the system Al-Co-Ni. Its structure contains the so-called “20 Å-cluster”, which is a characteristic building unit of decagonal Al-Co-Ni. The Co/Ni ratio determines which modification of decagonal  $\text{Al}_{72}\text{Co}_{28-x}\text{Ni}_x$  ( $8 \leq x \leq 20$ ) is formed. Therefore, we studied the influence of the Co/Ni ratio on the structure of the W-phase, starting from binary compositions Al-Co and Al-Ni with idealized positions. From these results a realistic ternary model will be derived.

The structure models were optimized using the VASP code [2,3]. Our calculations are based on the generalized gradient approximation and utilized PAW potentials [4] supplied with VASP. The band structure, electron density distribution and electron localization function were calculated.

These calculations help to get insight into the factors governing formation and stability of this kind of complex intermetallic alloy. They also corroborate the results of the single-crystal X-ray structure analysis, from which a significantly distorted and disordered structure model was obtained.

- [1] Sugiyama, K., Nishimura, S., Hiraga, K., *Jour. Alloys Comp.*, **2002**, 342
- [2] Kresse, G., Furthmüller, J., *Comput. Mat. Sci.*, **1996**, 6
- [3] Kresse, G., Furthmüller, J., *Phys. Rev. B*, **1996**, 54
- [4] Kresse, G., Joubert, J., *Phys. Rev. B*, **1999**, 59

### Honeycomb diffuse intensities in NaREF<sub>4</sub> upconversion materials

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Karl W. Krämer<sup>b</sup>, Thomas Weber<sup>c</sup>

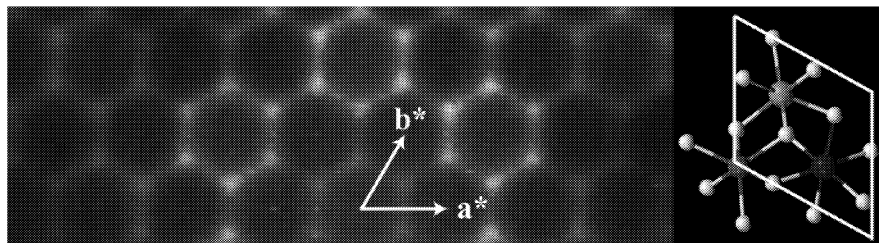
<sup>a</sup>Lab für Kristallographie, University of Berne, Switzerland

<sup>b</sup>Dept of Chemistry and Biochemistry, University of Berne, Switzerland

<sup>c</sup>Lab für Kristallographie, ETH Zurich, Switzerland

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Hexagonal sodium rare-earth (RE) fluorides, e.g. NaYF<sub>4</sub>: Yb, Er, are very efficient upconversion materials, which emit visible light upon infrared excitation. The efficiency of the upconversion process depends mainly on the doping ratio, the phase purity and the Na:RE ratio. These phases have hexagonal structures with a disordered cation distribution. Here we report a detailed investigation of Na<sub>1.5</sub>La<sub>1.5</sub>F<sub>6</sub>. The reconstructed layers of reciprocal space contain either sharp Bragg reflections for integer values of  $l$ , or planes with honeycomb-like diffuse intensities for half-integer values of  $l$  (Fig left:  $h k 1.5$ ). The Bragg reflections indicate a hexagonal metric and the average structure could be refined with space group symmetry  $P-6$ . It shows three different columns of cations with Na, La or a 1:1 ratio of both (Fig right). The diffuse intensities are well reproduced if it is assumed that Na and La alternate regularly in the disordered columns along  $c$  and that Na and La alternate with a probability less than one in the  $a, b$  plane.



## The new decagonal quasicrystal in the ternary system Al–Ir–Os

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8093 Zurich, Switzerland*

The ternary Al–Ir–Os decagonal phase with  $\sim 16.8$  Å periodicity was found in the as-cast as well as in the annealed samples in the composition range of about 80-81 at.% Al and 12-13 at.% Ir.

Preliminary studies of the rapidly solidified alloys in the binary systems Al–Ir and Al–Os show the presence of metastable decagonal  $Al_4Me$  [1, 2] quasicrystals (QC's). In the case of  $Al_4Ir$  authors report  $\sim 16$  Å periodicity along the tenfold rotation axis.

Some mutual combinations of the known metastable QC's in the binary systems Al–TM (TM=Co, Ni, Fe) [3, 4, 5, 6] show thermodynamically stable ternary decagonal phases [7, 8]. The aim of this work, besides its interest concerning phase equilibria, was to look for the existence, stability and structural features of ternary quasicrystalline phases in the Al–Ir–Os system.

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1. R. Wang, L. Ma and K.H. Kuo, *J. Less Common Met.*, 163 (1990) 27-35.
2. Z. Wang, Y. Gao and K.H. Kuo, *J. Less Common Met.*, 163 (1990) 19-26.
3. E. Abe, A.P. Tsai, *J. Alloys Comp.* 342 (2002) 96-100.
4. B. Grushko, D. Holland-Moritz, K. Bickmann, *J. Alloys Comp.* 236 (1996) 243-252.
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6. R. C. Henley, *J. Non-Crystall. Solids* **75** (1985) 91-96.
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## Anisotropic displacement parameters for normal mode analysis: Which refinement is needed?

Therese Lüthi Nyffeler<sup>a</sup>, Keiichiro Ogawa<sup>b</sup>, Hans-Beat Bürgi<sup>a</sup>

<sup>a</sup> *Laboratorium für Kristallografie, University of Berne, Switzerland*

<sup>b</sup> *Department of Chemistry, The University of Tokyo, Komaba, Japan*

Information on low-frequency modes of molecular motion in the crystal<sup>[1]</sup> can be extracted from Anisotropic Displacement Parameters (ADPs) measured over a wide range of temperatures. Here we investigate the bias on the ADPs due to effects of deformation density and its influence on the model of motion.

Four models were refined with a data set on (*E*)-2,2'-dimethylstilbene measured at 90 K to the high resolution of 0.41 Å<sup>[2]</sup>: 1) Spherical form factors 2) Multipole Parameters (MPPs) from a library<sup>[3]</sup> 3) MPPs fitted to a calculated charge density<sup>[4]</sup> 4) MPPs fitted to the experimental charge density. The ADPs from the different refinements differ by 0.00006 - 0.0017 Å<sup>2</sup>, corresponding to 1 to 20 s.u.. The U11 and U22 components lying in the molecular plane decrease for models 2, 3 and 4 as compared to model 1. The decrease is largest for model 4. In model 2 the U33-out of plane components are becoming clearly bigger whereas they become smaller with model 4 compared to a spherical model. In the Normal Mode Analysis these differences are reflected primarily in a decrease of the temperature-independent part of the model of motion<sup>[1]</sup>.

<sup>1</sup> H.B. Bürgi, S.C. Capelli, *Acta Cryst.* 2000, **A56**, 403-412.

<sup>2</sup> K. Ogawa, J. Harada, unpublished results.

<sup>3</sup> V. Pichon-Pesme, et al, *J. Phys. Chem.* 1995, **99**, 6242-6250.

<sup>4</sup> Courtesy of T. Koritsansky, Middle Tennessee State University.



## Unit cellmates: the *cis* and *trans* isomers of an iron(II) complex co-crystallize

Karl W. Törnroos<sup>a</sup>, Marc Hostettler<sup>b</sup>, Dmitry Chernyshov<sup>c,d</sup>,  
Hans-Beat Bürgi<sup>b</sup>

<sup>a</sup>*Department of Chemistry, University of Bergen, Norway*

<sup>b</sup>*Laboratory of Crystallography, University of Berne, Switzerland*

<sup>c</sup>*Petersburg Nuclear Physics Institute, Russia*

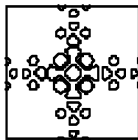
<sup>d</sup>*Swiss-Norwegian Beam lines at ESRF, Grenoble, France*

The crystal structure of dichloro-bis(2-picolyamine-iron(II)) contains a 1:1 ratio of the *cis* and *trans* isomers. The former lies on a two-fold axis whereas the latter lies on an inversion centre. The equatorial chlorine and NH<sub>2</sub> ligands of the two isomers lie in the same crystal planes exhibiting an intricate 2D hydrogen bond network with four eight-membered rings around each iron constructing a tiling pattern throughout the layer. These hydrogen bonded layers are interconnected through extended  $\pi$ - $\pi$  interaction between the axial pyridine ligands.

The number of crystal structures with co-crystallized isomers found in the CSD is very limited. In fact only one analogous, ordered example with *similar* ligand atoms (MN<sub>4</sub>Cl<sub>2</sub>) seems to exist.

The rare occurrence of this phenomenon may be understood intuitively from the facts that firstly, both isomers, which are expected to have different energies and most probably also different synthesis conditions, must happen to be present during crystallization, and that secondly, the formation of the co-crystal must be more favourable in thermodynamic and/or kinetic terms than the formation of crystals containing the individual isomers only.

[1] Zhu, D., Xu, Y., Yu, Z., Guo, Z., Sang, H., Liu, T. & You, X, *Chem. Mater.*, 2002, **14**, 838.



**SGK/SSCr Swiss Society for Crystallography**  
**SKT/SCT** Section for Crystal Growth and Crystal Technology

## General Assembly 2005

Thursday, October 13 at 17h00

### Agenda

1. Minutes of the Annual General Assembly in Neuchâtel on October 6, 2004  
(published in SGK/SSCr Newsletter 64)
2. Report from SGK/SSCr
  - Report of the President (R. Cerny)
  - Report of the Treasurer for 2004 (M. Hennig)  
(cf. SGK/SSCr Newsletter 64)
  - Report of the Auditors for 2004 (Ch. Bärlocher / K. Schenk)
  - Preliminary report of the Treasurer for 2005 (M. Hennig)
  - Presentation of the Budget 2006, Membership fee 2006 (M. Hennig)
3. Report from SKT/SCT
  - Report of the Section head (H. Scheel)
  - Report of the Treasurer for 2004 (K. Fromm)  
(cf. SGK/SSCr Newsletter 64)
  - Report of the Auditor for 2004
  - Preliminary report of the Treasurer for 2005 (K. Fromm)
  - Presentation of the Budget 2006 (K. Fromm)
4. Report of the delegates to the IUCr General Assembly (H. Grimmer / R. Cerny)
5. Report of the delegate to the ECA Council Meeting (H. Stoeckli-Evans)
6. Award of travel grants (R. Cerny)
7. International conferences in Switzerland related to crystallography (R. Cerny)
8. Election of the committee and the president of the SSCr for 2006-2008
9. Election of the delegate to the Senate of the Swiss Academy of Sciences and of his proxy
10. Election of the auditors
11. Next annual meeting of the SGK/SSCr (new President)
12. Varia

## Revisorenbericht für die Jahresrechnung 2004 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS	UBS	291-110.0
Credit Suisse	CS	913652-00
Postkonto	PC	30-532275-8

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2004 bis 31. Dez. 2004. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2004 ist der Stand der Konten und der Kasse:

UBS	SFr.	12'876.91
CS	SFr.	16'525.65
PC	SFr.	369.62
Kasse	SFr.	524.80

Die Unterzeichneten beantragen der Versammlung die Entlastung des Kassierers und der Revisoren für die geprüfte Periode.

Ort / Datum

Basel, 23. März 2005

Unterschriften

Ch. Bärlocher  
(ETH Zürich)

K. Schenk  
(EPF Lausanne)

## Candidates for the SSCr Committee 2006-2008

Candidate for President:

**Walter Steurer, Prof. Dr.**

Laboratory of Crystallography, Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse 10, 8093 Zurich

Tel: 01-632 6650, Fax: 01-632 1133, E-mail: steurer@mat.ethz.ch

Home page: <http://www.crystal.mat.ethz.ch/>

**Education:** Diploma (Chemistry, 1976); Ph.D. Univ. of Vienna (Physical Chemistry, 1979, specialisation: structural chemistry); Habilitation Univ. of Munich (Crystallography and Mineralogy, 1987).

**Positions:** Post-doc, Research Assistant and Lecturer at the Institute of Crystallography and Mineralogy (University of Munich, 1980-1992); Professor of Crystallography and Mineralogy (University of Hannover, 1992-1993); Professor of Crystallography (ETH and University of Zurich, 1993-present); calls to full professorships in Hamburg (1992) and Munich (1999) declined.

**Professional Activities:** Editor-in-chief of Zeitschrift für Kristallographie; Director of Studies of the Department of Materials Science of ETH Zurich; former Chairman of the Department of Earth Sciences of ETH Zurich; Member of: Swiss Society for Crystallography (SSCr), American Crystallographic Association (ACA), Materials Research Society (MRS), Deutsche Kristallographische Gesellschaft (DGK), Deutsche Mineralogische Gesellschaft (DMG), Deutsche Physikalische Gesellschaft (DPG).

**Research Interests:** Aperiodic crystals, higher-dimensional crystallography, crystallography at non-ambient conditions.

Candidate for Secretary:

**Schefer, Jürg, Dr.**

Laboratory for Neutron Scattering ETHZ & PSI, WHGA/146, CH-5232 Villigen PSI

Tel: 056-310 4347, Fax: 056-310 2939, E-mail: Jurg.Schefer@psi.ch

**Education:** Diploma in Physics (1979) and PhD in Physics (Dr. sc. nat. ETH, 1983) at ETH Zürich (Thesis work: Structural investigations on metal hydrides).

**Positions:** Research Assistant, ETH Zürich (1984); Senior Research Associate at the Structural Biology Laboratory of Brookhaven National Laboratory and Collaborator of the Biochemistry Department of Columbia, New York (1984-1987); Wissenschaftlicher Adjunkt at SIN/PSI Villigen; Group Leader of the Neutron Diffraction Group of the Laboratory for Neutron Scattering ETHZ & PSI (since 2002).

**Professional Activities:** Member of the Scientific Advisory Committee of ILL (5a, 1991-1996), member of the organizing committee of the first European Conference on Neutron Scattering in Interlaken (1991) and member of the program committee of the first neutron scattering summer schools in Zuoz, Engadin (1993), Editor of the PSI Scientific Reports of NUM/FUN (since 1998-2004).

**Research Interests:** Chemical and magnetic structure determination from single crystals (optical data storage materials, copperoxydes, ferromagnetics) using neutrons and X-ray diffraction.

Candidate for Committee Member:

**Michael Hennig, PD Dr.**

Pharma Research Basel Discovery, F. Hoffmann-La Roche Ltd., Grenzacherstr., CH-4070 Basel.

Tel: 061-6886046, Fax: 061-6887408, E-mail: Michael.Hennig@roche.com

**Education:** Crystallography and Biochemistry (Diploma, 1989); Ph.D. European Molecular Biology Laboratory (1992, protein crystallography); Post-doc, Charité Berlin (1992); Post-doc, Biozentrum, University of Basel (1993-1995); Habilitation in Protein Crystallography, Biozentrum, University of Basel (1997).

**Positions:** Research Assistant Biozentrum (Basel, 1993-1995), Lab-Head Crystallography F. Hoffmann - La Roche (Basel, 1995-2000), Group Leader Crystallography (2000-2001), Section Head Molecular Structure Research (2002-present).

**Professional Activities:** Member Deutsche Kristallographische Gesellschaft (DGK), Member Swiss Society for Crystallography (SSCr), Treasurer of the Swiss Society for Crystallography (2005-present).

**Research Interests:** Crystallography, X-ray powder diffraction, crystal polymorphism of drug substances, X-ray structure analysis of drug substances and proteins, structure-based drug design, investigation of protein-ligand interaction by X-ray and biophysical methods, physical methods for structure analysis of small molecules (MS, NMR, IR).

Candidate for Committee Member:

**Marc Schiltz, Prof. Dr.**

Laboratoire de Cristallographie, EPF Lausanne, EPFL-FSB-IPMC-LCR, Bât. BSP, CH-1015 Lausanne

Tel: 021-693 0631, Fax: 021-693 0504, E-mail: marc.schiltz@epfl.ch

Home page: <http://lcr.epfl.ch>

**Education:** Degree (Licence & Maîtrise) in Physical Chemistry, 1992, University of Paris VII; Ph.D. University of Paris XI-Orsay, 1997, specialisation: macromolecular crystallography.

**Positions:** Post-doc at the MRC Laboratory of Molecular Biology (group of G. Bricogne), Cambridge (UK), 1997-1998; Lecturer (Maître de conférences) at the University of Paris XI-Orsay and research assistant at LURE (Laboratoire pour l'Utilisation du Rayonnement Electromagnétique), 1999-2003; sabbatical leave as research scientist for Global Phasing Ltd., Cambridge (UK), 2002-2003; appointed Assistant Professor at the EPF Lausanne in November 2003.

**Professional Activities:** Member of: Swiss Society for Crystallography (SSCr), Association Française de Cristallographie (AFC) and Groupe Thématique de Biologie Structurale (GTBio).

**Research Interests:** Methods in macromolecular crystallography, applications of synchrotron radiation, experimental methods for phase determination, crystallographic computing, resonant diffraction in organic and biological crystals, radiation-induced transitions in organic and biological crystals, powder diffraction applied to bio-macromolecules.

Candidate for Committee Member:

**Klaus Yvon, Dr. Prof.**

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**Education:** PhD (Physics, 1967, University of Vienna)

**Positions:** Postdoctoral Research Fellow (University of Pennsylvania, Philadelphia, 1967 – 1970); Chargé de Recherche and Assistant Professor (Université de Genève, 1970 – 1982); Full Professor (Crystallography, Université de Genève, since 1982); Invited Professor (Max-Planck-Institut für Festkörperforschung Stuttgart, in 1979, and Université de Paris Sud, in 1995 and 1996); Sir Allan Sewell Fellow (Griffith University, Brisbane, in 2000); calls to full professorships in Bayreuth (1989) and Graz (1990) declined.

**Professional activities:** Head of Crystallography Laboratory, University of Geneva (since 1989); President of the Swiss Society of Neutron Scattering (1998-2000); Chairman of the Scientific Council of the Institute Laue-Langevin, Grenoble (1997-2000); Chairman of the Scientific Council of the Swiss Neutron Spallation Source SINQ at Paul-Scherrer Institute (1995-2000); Member of the Scientific Advisory Committee (1995-1998) and Council Member (1999-2002) of the European Synchrotron Radiation Facility; Member of the Steering Committee of the Centre for Study of Energy Problems at University of Geneva (1989-1997); Member of the International Steering Committee of the Conference Series: International Symposium on Metal-Hydrogen Systems, Fundamentals and Applications (since 1998), International Conference on Solid Compounds of Transition Elements (since 1996), and HYPOTHESIS (Hydrogen Power - Theoretical and Engineering Solutions, since 2003); member of numerous national and international Scientific Societies.

**Research interests:** Synthesis, structure analysis and physical properties of intermetallic compounds and new hydrogen storage materials.

## News of Members

**We welcome the following new member of the SGK/SSCr:**

**Ekaterina Pomjakushina** (Labor für Entwicklung und Methoden, Festkörperforschung mit Neutronen und Myonen, Paul Scherrer Institut, Villigen)

**Howard Flack** and **Hans Grimmer** have been elected members of the "Commission on Mathematical and Theoretical Crystallography" of the IUCr.

**Anthony Linden** at the Institute of Organic Chemistry of the University of Zurich completed his habilitation and became a Privatdozent as of July 2005.

**Artem R. Oganov** (ETH Zurich) has been offered tenure-track Assistant Professorship at Princeton University. He declined this offer for personal reasons and will continue building his Computational Crystallography Group at ETH Zurich.

**Artem R. Oganov** and his undergraduate research student, C.W. Glass, have developed a new method for crystal structure prediction. This method, based on quantum-mechanics, is the basis of the USPEX code written by Glass and Oganov. USPEX method allows one to predict crystal structure of any given material at any given P-T conditions on the basis of chemical composition alone. In its current form, the method is very fast and reliable for systems containing up to 30 atoms in the unit cell, but new developments that are underway will enable prediction of crystal structures even with hundreds of atoms in the cell. Principles and results of this method have been presented by Oganov and Glass at the IUCr meeting in Florence.

**Helen Stoeckli-Evans** (Université de Neuchâtel) has been promoted to Prof. Extraordinaire from the 1<sup>st</sup> of October 2005.

## News from the IUCr

The twentieth General Assembly of the IUCr, held in Florence, Italy, 23-30 August 2005 elected the following new Executive Committee:

President:	Y. Ohashi (Japan)
Vice-President:	I. Torriani (Brazil)
General Secretary and Treasurer:	S. Lidin (Sweden)
Past President:	W.L. Duax (USA)
Ordinary members:	P. Colman (Australia)
	G.R. Desiraju (India)
	C. Gilmore (UK)
	G. Heger (Germany)
	C. Lecomte (France)
	D. Viterbo (Italy)

## Venues of future European Crystallographic Meetings (ECM) and IUCr Congresses:

ECM 2006	Leuven (Belgium)
ECM 2007	Marrakech (Morocco)
IUCr 2008	Osaka (Japan)
ECM 2009	Istanbul (Turkey)
ECM 2010	Darmstadt (Germany)
IUCr 2011	Madrid (Spain)

Thesis submitted to the University of Basel by Adeline Y. Robin  
in the group of Prof. Katharina M. Fromm

(Date of the examination: 26 July 2005)

## Structural Diversity of Cu(I), Cu(II) and Ag(I) coordination polymers with the ligand ethanediy bis(isonicotinate)

The interest in the construction of coordination polymers by linking transition metal ions with polydentate ligands has been constantly growing over the past years. The infinite frameworks are obtained by self-assembly of various building blocks connected by weak interactions: metal ion coordination as well as hydrogen bonds,  $\pi$ -interactions, and metal-metal interactions are possible components in the construction of supramolecular structures. The study of the crystallographic structures of these metal-organic frameworks represents an essential point in the understanding of the network formation.

In this context, several coordination polymers were synthesized based on the ligand ethanediy bis(isonicotinate) and Cu<sup>I</sup>, Ag<sup>I</sup> or Cu<sup>II</sup> salts as metal components [1]. The aim of this thesis is the study of the behaviour of this ligand and the related cations under several conditions: use of different solvents or counter ions. The crystallographic study allows us to characterize and analyse the obtained coordination polymers, and especially to compare the compounds.

### Ligand

The ethanediy bis(isonicotinate) (**L**) is formed by two pyridine rings linked by a flexible bridge containing two ester functions.



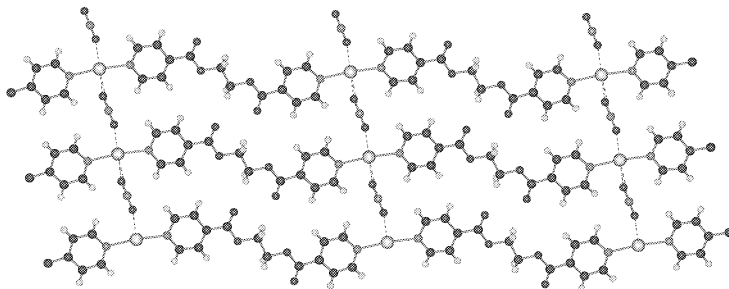
Due to its flexibility the ligand can adopt two different conformations: the "anti-" and the "gauche-" one, as drawn above.

### Copper(I) Chloride Coordination Polymers [2]

Under different solvent conditions, the compounds  $\{[\text{CuCl}(\text{L})]\cdot 0.5\text{THF}\}_n$  and  $\{[\text{CuCl}(\text{L})]\}_n$  can be crystallized. The presence of co-crystallized tetrahydrofuran (THF) molecules induces the formation of a double chain motif with the bending of the ligand, whereas the motif in  $\{[\text{CuCl}(\text{L})]\}_n$  is a linear chain with the anti-conformation of the ligand. Moreover, it seems that  $\{[\text{CuCl}(\text{L})]\cdot 0.5\text{THF}\}_n$  can be transformed into the solvent-free form by elimination of the THF molecules and formal cutting of several bonds, followed by a rearrangement of the ligand. This transformation is solvent-mediated, as it occurs in solution.

### Silver(I) Coordination Polymers

*Counter ions' influence:* The use of triflate, perchlorate, hexafluorophosphate or nitrate as counter ions for the building of Ag<sup>I</sup> coordination polymers shows the preference for silver to adopt a linear geometry when coordinated by bidentate *N,N'*-donors ligands. The counter ions influence mostly the long range arrangements of the motifs.



The coordination polymer  $\{[Ag(L)](NO_3)\}_n$ : linear chains ...-Ag-L-Ag-L-Ag... stacked parallel to each other with the nitrate counter ion as linker between them.

*Solvents' influence:* The building of silver nitrate coordination polymers in different solvents (*i.e.* THF/ethanol, acetonitrile or THF/water) reveals a correlation between the silver nitrate solubility and the final Ag–O(nitrate) distances in the solid state structure. *Water-content dependent variations in the structure of  $\{[Ag(L)](NO_3)(H_2O)_x\}_n$  ( $x=0,1,2$ )* [3]: The three compounds are concomitant polymorphs grown in a solvent mixture (THF/water). Without water in the crystal structure, simple one-dimensional chains are obtained. As soon as water co-crystallizes, the good solvating capacity of water towards the nitrate anions is revealed by H-bonding interactions between nitrate and water. This induces drastic structural changes with, especially, the apparition of short Ag-Ag contacts and pairing of the chains.

### Copper(II) Coordination Polymers

The coordination polymers obtained from copper nitrate or copper perchlorate show one-dimensional motifs, even if motifs of higher dimensionality are expected with the use of Cu<sup>II</sup> as cation.

This structural study of the behaviour of the ligand ethanediy bis(isonicotinate) with copper and silver ions during coordination polymer construction is the preliminary step before the use of such systems in further investigations: long-range magnetic ordering in low-dimensional metal complexes, introduction of further cations, formation of thin films by layer-by-layer deposition, etc. This work is furthermore an important contribution to the highly interesting problem of structure prediction, polymorphism studies and crystal engineering.

[1] K.M. Fromm, R. Bergougnant, W. Maudez, A.Y. Robin, J. Sagué. *Z. Anorg. Allg. Chem.*, **2005**, 631, 1725-1740.

[2] A.Y. Robin, K.M. Fromm, H. Goesmann, G. Bernardinelli. *Cryst. Eng. Comm.*, **2003**, 5, 405-410.

[3] A.Y. Robin, M. Meuwly, K.M. Fromm, H. Goesmann, G. Bernardinelli. *Cryst. Eng. Comm.*, **2004**, 6, 336-343.



**Swiss Spallation Neutron Source SINQ**  
**Swiss Synchrotron Light Source SLS**  
**Swiss Muon Source SμS**

## Calls for proposals

The Paul Scherrer Institute, Villigen, CH (<http://www.psi.ch>) operates three major user laboratories for condensed matter research on one campus: a third generation X-ray synchrotron source (SLS), the only continuous spallation neutron source worldwide (SINQ) and the world's most powerful continuous-beam  $\mu$ SR facility (SμS).

Please remember the following proposal submission deadlines:

**SLS:**

Protein crystallography beamlines : 15/02, 15/06, 15/10  
 All other beamlines : 15/03, 15/09

**SINQ:**

All instruments : 15/05, 15/11

**SμS:**

All instruments : 01/12

The central PSI User Office offers a joint Web portal, from where all necessary information can be obtained: <http://user.web.psi.ch>

**Contact address:**

Paul Scherrer Institut  
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 CH-5232 Villigen PSI

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 Fax : +41-56-310 3294  
 Web : <http://user.web.psi.ch>

E-mail: [slsuo@psi.ch](mailto:slsuo@psi.ch), [sinq@psi.ch](mailto:sinq@psi.ch), [smus@psi.ch](mailto:smus@psi.ch)

## Calendar of Forthcoming Meetings

**Meetings held in Switzerland are printed in bold letters.**

More details on most meetings can be found on the WWW under

<http://www.ch.iucr.org/iucr-top/index.html>

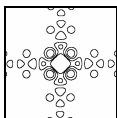
2005

<b>10. – 18. Sept.</b>	<b>Beatenberg (Switzerland)</b>	<b>3<sup>rd</sup> International Workshop on Crystal Growth Technology (IWCGT-3)</b>
15. – 17. Sept.	Murnau (Germany)	Structural Biology of Molecular Recognition
<b>19. – 21. Sept.</b>	<b>Les Diablerets (Switzerland)</b>	<b>2005 Swiss Workshop on Materials with Novel Electronic Properties MaNEP</b>
22. – 23. Sept.	Berlin (Germany)	13 <sup>th</sup> BENSU Users' Meeting
29. – 30. Sept.	München (Germany)	Kurs "Neutronenstreuung für Kristallographen" des AK Neutronenstreuung der DGK
<b>3. – 7. Oct.</b>	<b>Villigen (Switzerland)</b>	<b>4<sup>th</sup> NCCR Practical Course – Synchrotron Data Acquisition Techniques in Macromolecular Crystallography</b>
4. – 7. Oct.	Hofgeismar (Germany)	Fortbildungskurs: Anwendung der Gruppentheorie in der Kristallchemie
6. – 7. Oct.	Stuttgart (Germany)	Watching the Action: Powder Diffraction at Non-Ambient Conditions
10. – 14. Oct.	Hamburg (Germany)	Autumn School: Application of Neutron and Synchrotron Radiation in Engineering Materials Science
<b>13. October</b>	<b>Lausanne (Switzerland)</b>	<b>Annual Meeting 2005 of the SGK/SSCr "Crystallography and Physics"</b>
<b>17. – 18. Oct.</b>	<b>Villigen (Switzerland)</b>	<b>6<sup>th</sup> SLS Users' Meeting</b>
<b>18. – 20. Oct.</b>	<b>Villigen (Switzerland)</b>	<b>XRMS 2005: X-Ray Spectroscopy of Magnetic Solids</b>
<b>24. – 27. Oct.</b>	<b>Villigen (Switzerland)</b>	<b>ROG 2005: International Workshop on Reflectometry, Off-specular Scattering and GISANS</b>

30. Oct. – 3. Nov.	Beijing (China)	Recent Advances in Phasing Methods for High-Throughput Protein Structure Determination
3. – 5. Nov.	Argonne (USA)	63 <sup>rd</sup> Pittsburgh Diffraction Conference
27. Nov. – 2. Dec.	Sydney (Australia)	International Conference on Neutron Scattering 2005

2006
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<b>25. – 27. January</b>	<b>Villigen (Switzerland)</b>	<b>SμS Users' Meeting</b>
20. – 23. February	Limoges (France)	6 <sup>ème</sup> Colloque Rayons X et Matière (RX 2006)
3. – 6. March	Freiburg (Germany)	14. Jahrestagung der DGK
13. – 24. March	Jülich (Germany)	10 <sup>th</sup> Laboratory Course: Neutron Scattering
<b>10. May</b>	<b>Villigen (Switzerland)</b>	<b>8<sup>th</sup> SINQ Users' Meeting</b>
9. – 18. June	Erice (Italy)	The Structure Biology of Large Molecular Assemblies
22. – 27. July	Honolulu (USA)	The American Crystallographic Association Annual Meeting
4. – 6. August	Leuven (Belgium)	Satellite Conference of ECM-23 on "Mathematical and Theoretical Crystallography"
6. – 11. August	Leuven (Belgium)	23 <sup>rd</sup> European Crystallographic Meeting (ECM-23)
28. August – 2. Sept.	Nancy (France)	Summer School: Analyse structurale par diffraction des rayons X, cristallographie sous perturbation
<b>1. – 4. Sept.</b>	<b>Genève (Switzerland)</b>	<b>10<sup>th</sup> European Powder Diffraction Conference (EPDIC-X)</b>
25. – 28. Sept.	Berlin (Germany)	6 <sup>th</sup> International Workshop on Polarised Neutrons in Condensed Matter Investigations



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

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## **SGK/SSCr Newsletter**

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