



Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Società Svizzera di Cristallografia
Swiss Society for Crystallography

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



SGK / SSCr NEWSLETTER

ISSN 1662-5358 (printed edition)

ISSN 1662-534X (electronic edition)

No. 112
August 2024



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The President's Page



Dear members,

nearly three years have now passed since I wrote my first message to you as president of

the SSCr. At the time, it was my ambition to energize, maybe rejuvenate certain aspects of our society. We went to work on this with a largely reformed board, and, in retrospective, I am not unhappy about what we have achieved. We have been quite involved in different ways beyond administering the Society, which includes revamping our outreach and the creation of an annual workshop, something very dear to me. We have managed to maintain good diversity in the Flack Lectures and have been involved in the creation and organization of numerous international events. Creating, designing and realizing new activities is exciting and “easy” when carried by good vibes, harmony and motivation of the involved. I am optimistic that many of these recent initiatives will see stabilization now and (hopefully) longevity, albeit a somewhat harder task for the next presidency.

Throughout these past years a wave of positivity and enthusiasm has been continuously kept alive by the fantastic team on our board. Thank you, Paula, Dubravka, Olha, Enrico, Antonio, Nicola, Simon and Céline for defining, elaborating and realizing many SGK / SSCr Newsletter No. 112 (2024)

objectives while always working for the same cause. Perhaps it goes without saying, but should still be said, that you all spend much of your free time running the society, and that the Swiss community is lucky to have such an active and committed group of colleagues working for them. Thank you to all the members for your trust and your participation to our events and activities.

We are coming to Basel this year on September 12th, for our annual meeting. On this occasion, we will be electing a new president. There is still much in the pipeline for the current board and I wish our new president all the best.

These have been three very formative years for me, and much has been learnt for the future. It has been a real pleasure to serve the Swiss crystallographic community, and I hope to have done a decent job at it. More than ever, I am reminded to appreciate societies, associations, groups and the like, which make up a strong, rich and significant part of Swiss culture and society. Give them a try if you have not yet. My message ends by encouraging you one last time as president to join, contribute and help out to maintain a stable and thriving crystallographic community in our country!

I look forward to seeing many of you during the summer conferences and at our annual meeting in Basel. My best wishes to all of you.

Pascal Schouwink

Program Annual Meeting Swiss Society for Crystallography



11 September 2024

20:00-22:30 Conference Dinner [Hotel ODELYA](#) Missionsstrasse 21a CH-4055 Basel



[Switzerland Innovation Park](#) Hegenheimermatt 167
4123 Allschwill, Switzerland



12 September 2024

09:00 – 10:00		Registration, posters & coffee
10:00 – 10:10	Alessandro Prescimone	Welcome Address
10:10 – 11:40	Chairs: Tba	Applied Crystallography
10:10 – 10:50	Invited Speaker: Birger Dittrich (Novartis)	Crystal Structure Prediction & the value of crystal structures
10:50 – 11:10	Emilia Götz (Rigaku)	Variable temperature diffraction and polymorph screening with the XtaLAB Synergy-ED
11:10 – 11:30	Gwilherm Nénert (Malvern)	Crystal structure, polymorphism and re-entrant phase transition in NaSrPO ₄
11:30 – 12:00		Posters , sponsors, and Eldico lab visit
12:00 – 13:30		Lunch , posters and sponsors
12:40-13:30	for SSCr members	SSCr Annual General Assembly
13:30 – 14:50	Chairs: Tba	Biological Crystallography
13:30 – 14:10	Invited Speaker: Peter Wood (CCDC)	Polymorphism analysed: The evolution of solid form risk assessment using structural informatics
14:10 – 14:30	Dan Stefanita (Empa)	Multimodal X-ray methods to understand drug release mechanisms in local antibiotic therapy with calcium sulfate
14:30 – 14:50	Rohan Pokratath (Excelsus)	Streamlining the Pair Distribution Function Analysis of Pharmaceutical Molecular compounds
14:50 – 15:20		Coffee break, posters and sponsors
15:20 – 17:30	Chairs: Tba	Chemical Crystallography
15:20 – 16:00	Speaker: Simon Parsons (University of Edinburgh)	Thermodynamics of Compression in Molecular Solids
16:00 – 16:20	Felix Eder (Uni Geneva)	Incommensurately modulated KCr _{1-x} Se ₂
16:20 – 16:40	Kanghyun Chu (Uni Bern)	Periodic Hirshfeld Atom Refinement
16:40 – 17:30		Poster prize and farewell apéro

Abstracts of the SGK / SSCr Annual Meeting 2024



Talk (40 min)

Crystal Structure Prediction & the value of crystal structures

B. Dittrich

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The presentation will provide an overview of the current state of Crystal Structure Prediction (CSP) as applied in the pharmaceutical industry and will cover the following aspects:

Use-case

Historical overview

The winning methodology emerging from CSP blind tests

Interpretation of Energy versus Density plots (landscapes)

Interpretation of DH as polymorphism risk

The role of disorder and high pressure in energy ranking

Structure solution from powder diffraction via CSP

CSP and NMR-crystallography

Form stability under real-world conditions

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Talk (40 min)

Polymorphism analysed: The evolution of solid form risk assessment using structural informatics

Peter Wood

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As the field of solid form informatics (1) has developed, particularly as applied to solid form risk assessment, so have the software approaches to support this kind of analysis. In 1998, Dr Eugene Sun, a research director at Abbott Laboratories, said about polymorphism: “we know that it will probably happen, but not why or when” (2).

In the 2000s, as research scientists, we had very limited specialist functionality to explore these topics and were mostly using searching in ConQuest to uncover key factors that might influence polymorphism. In the 2010s, we started more actively using the relative 3D geometry of interactions, compared to IsoStar plots, to assess whether an interaction was “usual” or not, similarly we could look at interaction pairings based on likelihoods with Motif searching in Mercury, and the relative “usualness” of molecular geometry using Mogul. Now in the 2020s, we have much more automated, effective, and validated approaches to get straight to actionable insights.

This presentation will showcase the evolution of research approaches and software over the years in the field of solid form risk assessment, highlight the key role played in this evolution by the Crystal Form Consortium (CFC) a partnership with leading industrial organisations, and show the impacts of that evolution using some specific polymorphism examples.

As the proverb says: “If you want to go fast, go alone. If you want to go far, go together”.

References

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Talk (40 min)

Thermodynamics of Compression in Molecular Solids

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High pressure is a very useful means for studying the mechanical properties of intermolecular interactions. The effects of pressure on the Gibbs free energy of a solid involve changes in intermolecular interaction energies, volume, and entropy. Intermolecular interaction energies are usually calculated either by semi-empirical techniques, such as the Pixel method,^{1,2} or using periodic density functional theory. However, this talk will also demonstrate how they can be accessed experimentally. Volume minimization is the dominant driving force in almost all high-pressure phase transitions. Therefore, the analysis of volume changes is critical in interpreting the thermodynamics consequences of high pressure. We have developed a Monte Carlo algorithm for the calculation of occupied ('network') and unoccupied ('void') space in crystal structures. The variation of the volumes of the voids and the network of intermolecular contacts with pressure sensitively reveals how pressure is accommodated by different parts of a structure (Fig. 1). Entropy changes as the energies of vibrations are affected by compression; these too can be calculated or measured experimentally. Though fewer data are available on this aspect of compression, particularly in molecular solids, it may be critical in stabilizing crystal structures with weak interactions.

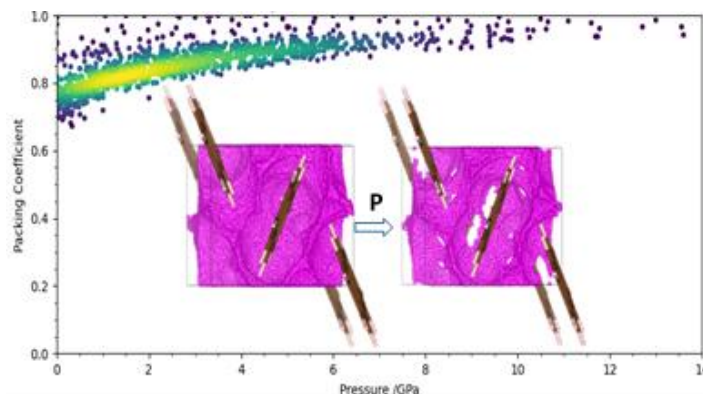


Figure 1. Variation of packing coefficient with pressure. Inset: loss of interstitial void space in naphthalene at high pressure.

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Talk (15 min)

Variable temperature diffraction and polymorph screening with the XtaLAB Synergy-ED

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Since its launch in 2021, the XtaLAB Synergy-ED has produced many structures, with over 400 unique structures from Rigaku labs alone. While most of these structures were analyzed at ambient temperature, recent advances in low-temperature techniques, particularly cryo-transfer, have proven invaluable for the preservation of sensitive samples both those sensitive to vacuum and those sensitive to electron beam damage. Additionally, the instrument's enhanced automation capabilities, such as queueing, have opened new avenues for polymorph screening.

The XtaLAB Synergy-ED's compatibility with existing TEM instrument holders provides structural scientists with the ability to conduct various experiments traditionally performed in X-ray crystallography. Cryo-transfer specimen holders, such as the Gatan ELSA, protect samples prior to vacuum introduction (1), enabling the study of solvates and other vacuum-sensitive species, and allowing for the investigation of phase behaviour. Examples of crucial findings made possible by cryo-transfer will be discussed.

Furthermore, the Hummingbird Scientific MEMS biasing/heating holder allows for the increase in temperature, facilitating the exploration of polymorphism of structures such as porous materials. Recent studies utilizing single-crystal data from electron diffraction on a MOF system, $\text{Cu}(\text{ta})_2$ (Hta=1*H*-1,2,3-triazole), have yielded significant insights at both room temperature and 200°C. These findings are compared with previous studies by Grzywa et al. (2012) using SC-XRD and PXR, demonstrating the instrument's capability in polymorphism research.

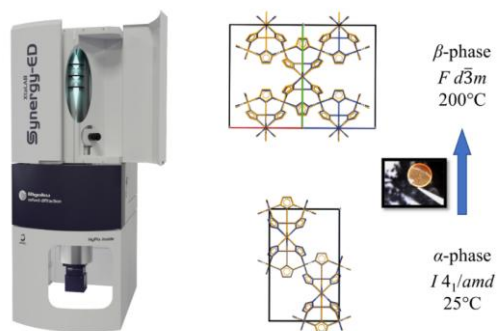


Figure 1 Overlays of the ambient and high temperature phases of $\text{Cu}(\text{ta})_2$ from the XtaLAB Synergy-ED (blue) and the X-ray structures by Grzywa *et al.* (orange).

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Talk (15 min)

Crystal structure, polymorphism and re-entrant phase transition in NaSrPO_4

Gwilherm Nénert

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The crystal chemistry of $\text{A}^{\text{I}}\text{B}^{\text{II}}\text{XO}_4$ (A^{I} = Alkali ion, B^{II} = alkali-earth ion, $\text{X} = \text{P}, \text{V}, \text{As}$) is very rich and has been widely investigated, particularly the phosphate family [1]. In recent years, we have been investigating the crystal structures [2,3] and magnetic properties of some compositions within the $\text{A}^{\text{I}}\text{B}^{\text{II}}\text{XO}_4$ series [4]. Besides the pure interest from a crystal chemistry point of view, the research activity related to this series of materials is driven mainly due to their ferroelectric, ferroelastic properties and possible applications as phosphors for LEDs [1, 5]. Within the rich $\text{A}^{\text{I}}\text{B}^{\text{II}}\text{VO}_4$ sub-family ($\text{X} = \text{V}$), we have recently found a new structural type: the larnite structure with the composition NaSrVO_4 [3]. In this contribution, we are investigating its counter phosphate composition. Despite its simple chemistry NaSrPO_4 has never been reported so far. Here, we present the synthesis, crystal structure and phase transitions of this phosphate. Surprisingly, this material exhibits a complex structure (31 atoms in the asymmetric unit-cell, $Z = 10$) at room temperature characterized by a strongly under bonded Na atom. This under-bonded atom is responsible for the complex and rich phase diagram as function of temperature as illustrated in Fig. 1. NaSrPO_4 exhibits 4 phase transitions between room temperature and 750°C . Besides its rich phase diagram, NaSrPO_4 exhibits a re-entrant phase transition slightly below 600°C before to reach a hexagonal paraelastic phase at high temperature. In addition, we show that the sequence of phase transitions is strongly driven by the history of the sample and several phases can be quenched at room temperature. Finally, the co-existence of Na channels within the structure with weakly bounded Na atoms makes this material a likely candidate for ionic conductivity.

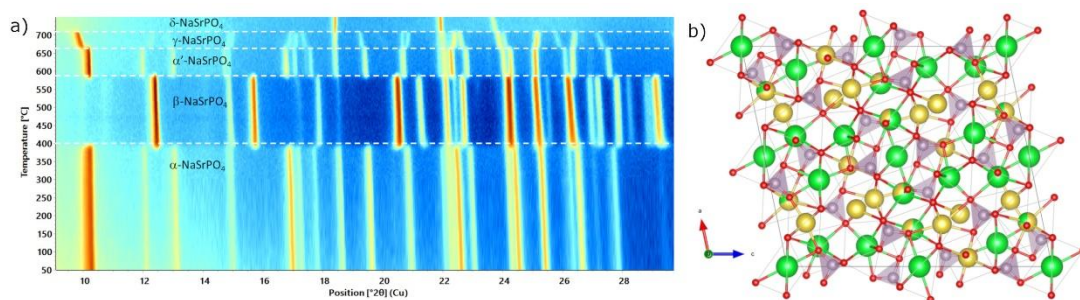


Figure 1: a) Temperature phase diagram of NaSrPO_4 and b) crystal structure of the α re-entrant polymorph.

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Talk (15 min)

Multimodal X-ray methods to understand drug release mechanisms in local antibiotic therapy with calcium sulfate

Dan Stefanita^{1,2}, Sabrina L. J. Thomä¹, Emanuel Gautier³, Peter Wahl^{4,5}, Antonia Neels^{1,2}

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(2) Department of Chemistry, University of Fribourg, Switzerland

(3) Department of Orthopaedic Surgery, HFR Fribourg-Cantonal Hospital, Switzerland

(4) Division of Orthopaedics and Traumatology, Cantonal Hospital Winterthur, Switzerland

(5) Faculty of Medicine, University of Bern, Switzerland

The treatment of infections in orthopaedic and trauma surgery remains a significant challenge in modern medicine. Local antibiotic treatment plays a primordial role in treating bone and joint infections^[1,2], increasing drug availability at the site of infection while reducing systemic toxicity. Calcium sulfate (CaSO_4) as an interesting carrier material, as it dissolve within the desired treatment duration and is soft enough not to cause relevant damage to prosthetic joint components. This study investigates the structural and morphological interaction of various antibiotic drugs (vancomycin^[1], tobramycin and ceftriaxone^[2]) with CaSO_4 as they have differing release kinetics. The primary objective is to gain a comprehensive understanding of the binding mechanisms of the antibiotic compounds within the CaSO_4 crystal structure. By exploring drug release kinetics and cellular uptake we aim to improve antibiotic delivery and clinical outcome in orthopaedic infections. This research seeks to understand how the antibiotic incorporation affects the crystalline matrix of CaSO_4 and how these interactions influence the overall performance of the drug delivery system. Our approach combines a multiscale approach^[3] of powder X-ray diffraction (PXRD) and pair distribution function analysis (PDF) as basic methods, completed by the advanced calculation techniques of density functional theory (DFT)^[4]. DFT provides information on surface adsorption energies and investigates forces such as chemical bonds, van der Waals interactions, and hydrogen bonds. Integrating experimental and computational approaches, this research aims to elucidate the mechanisms coordinating drug-carrier interactions and release profiles, potentially leading to improved local antibiotic delivery systems for orthopaedic infections.

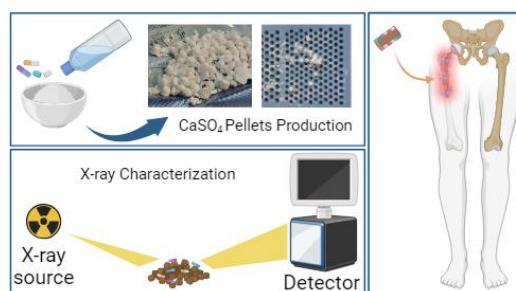


Fig. 1 Summary of sample preparation, analysis and treatment procedure.

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Talk (15 min)

Streamlining the Pair Distribution Function Analysis of Pharmaceutical Molecular compounds

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Pair distribution function (PDF) analysis is a powerful technique used to investigate the atomic-scale structure of materials by examining the distribution of interatomic distances. This method provides detailed insights into both crystalline and amorphous states, which is essential for understanding their physical properties, interactions, and behaviours. Applying PDF analysis to pharmaceutical molecular compounds involves several critical steps and challenges.

The primary challenge lies in generating a reliable PDF curve. This is particularly critical when using PDF for qualitative analysis of pharmaceutical powders, but it can also influence the development of PDF refinements. The process begins with meticulous sample preparation, including the selection of appropriate sample containers, generally capillaries. X-ray diffraction data must then be collected using an optimal setup and instrumentation to capture the necessary details. The scattered intensity in powder patterns of low-Z compounds, such as pharmaceuticals, rapidly decays due to their intrinsically weak and rapidly decaying structure factor. This suggests the use of medium photon energy and a wider 2theta angular range equivalently acceptable set up than higher photon energy and a narrower theta angular range. However, with low-Z materials backscattering from sample environment and experimental setup can often dominate the high-Q signal and the use of high energy photons allowing us to contain the reciprocal space of interest below 90 degrees, eliminates this potential source of error. Subsequently, the data undergo sophisticated reduction methods, including background subtraction, normalization, and corrections to produce accurate pair distribution functions. Data reduction must account for noise and extrinsic signals, a particularly challenging task for amorphous samples with less defined peaks. It often difficult to reproduce the data precisely with different setups.

Here, we present a comprehensive approach to performing meaningful PDF analysis of pharmaceutical molecules by streamlining the process from sample preparation to modelling. We demonstrate how this can be achieved across various pharmaceutical compounds and suggest optimal practices for each step. By addressing current challenges and leveraging recent advances in PDF techniques, particularly in the data collection/reduction methods, we aim to further enhance the understanding of pharmaceutical molecules, thereby improving drug design and development.

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Talk (15 min)

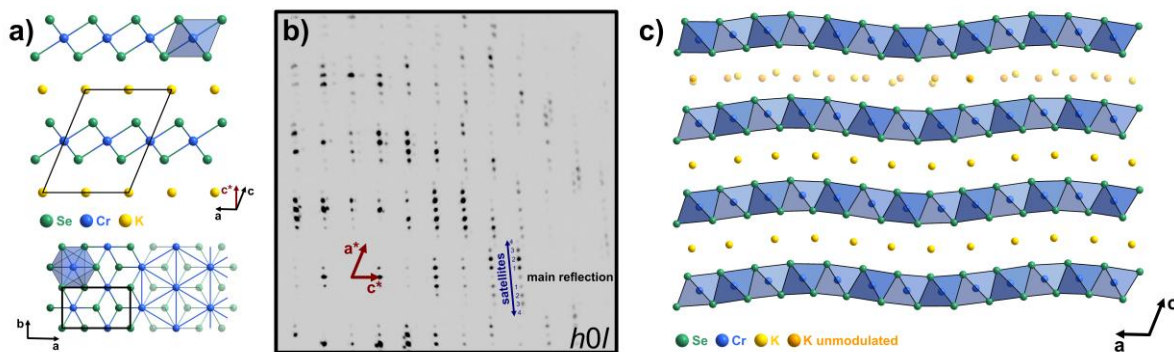
Incommensurately modulated $\text{KCr}_{1-x}\text{Se}_2$

Felix Eder*, Catherine Witteveen, Enrico Giannini, Fabian O. von Rohr

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Magnetic van der Waals materials receive booming interest, since their exfoliability down to the atomic limit allows for the exploration of 2D magnetism. One prominent member of this family, CrSe_2 , is commonly synthesized by oxidative deintercalation of KCrSe_2 (1). Like several other ACrX_2 phases, KCrSe_2 crystallizes in the delafossite structure type, consisting of $[\text{CrSe}_2]$ layers intercalated by K cations in a trigonal-rhombohedral stacking.

Using a mixed K-Se flux method, we were able to grow large single crystals of under-stoichiometric $\text{K}_{1-x}\text{CrSe}_2$ ($x \approx 0.13$). The basic structure of $\text{K}_{1-x}\text{CrSe}_2$ ((a), $C2/m$; $a = 6.3489(4) \text{ \AA}$, $b = 3.75881(14) \text{ \AA}$, $c = 8.2224(6) \text{ \AA}$, $\beta = 112.536(9)^\circ$, $V = 181.24(2) \text{ \AA}^3$) consists of the same structural features as KCrSe_2 . However, as manifested by intense satellite reflections in single crystal X-ray diffraction measurements (b), it is modulated by an incommensurate modulation vector $\mathbf{q} = 0.2675(4)\mathbf{a}^* - 0.1585(4)\mathbf{c}^*$. The size of the modulation vector is independent of temperature in the range of 90–350 K but slightly varies between different crystals of the same batch. The resulting crystal structure was solved and refined against the main reflections and satellites up to fourth order in the 3+1 dimensional super space group $C2/m(a0g)00$ with Jana2020 (2) to $R1_{\text{obs}} = 3.12 \%$ and $wR2_{\text{all}} = 8.33 \%$.



The under-occupation of the K cations is the driving force of the modulation, and the K content can be determined from the q_1 component of the modulation vector. The crystal structure compensates for the mismatch between the translational periods of $[\text{CrSe}_2]$ layers and K cations with an undulation of the layers (c), which hasn't been observed for any other ACrX_2 phases, but for in a similar way for $\text{Na}_{0.78}\text{CoO}_2$ (3). Supported with EDS and anisotropic magnetization data, this talk will work out the differences between $\text{K}_{1-x}\text{CrSe}_2$ and KCrSe_2 and attempt to explain them based on simple structural and chemical considerations.

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Talk (15 min)

Periodic Hirshfeld Atom Refinement

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Hirshfeld atom refinement (HAR) is an advanced technique for the determination of structural parameters in single-crystal X-ray diffraction experiments. This method relies on aspherical atomic form factors, which are obtained by partitioning the electron density provided by *ab initio* quantum chemical calculations. This approach was successful in molecular crystal systems but faced difficulties when applied to network compounds---any choice of their unit cell fails to have a stable free-standing configuration, and the partitioned electron density of each constituent atom is far from the reality.

To overcome this limitation, a new approach for periodic HAR is developed. It is applicable to network compounds such as silicate minerals, as well as molecular salts with strong intermolecular interactions. This is achieved by combining the open-source quantum crystallographic program *Tonto*(1) and the commercially available package for periodic calculations *Crystal23*(2) through the interface software *lamaGOET*(3). Each iteration involves calculating the electron density of a unit cell using *Crystal23*, partitioning the obtained electron density with *Tonto*, and optimizing the structure parameters to best match the diffraction data again using *Tonto*. This process is repeated until all the structural parameters are converged. This technique opens new pathways for accurately exploring a wider range of crystal systems from a structural point of view.

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Poster

Insights into the Bonding Nature of Arsenic, Phosphorus, and Sulphur Ylides: an answer from quantum crystallography

Yaser Balmohammadi¹, Lorraine A. Malaspina¹, Simon Grabowsky^{1*}

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Ylides are a class of chemical compounds classified as zwitterion by having a positively charged atom directly attached to a negatively charged atom. The most common types of ylides involve a positively charged heteroatom like nitrogen, phosphorus, sulphur, or arsenic attached to a negatively charged carbon atom. [1,2] Ylides are textbook examples of the interplay between Lewis resonance forms and molecular reactivity/function. Phosphorus ylides or phosphonium ylides have been widely used in organometallic and organic synthesis, most famously as Wittig reagents in the Wittig reaction. Sulphur ylides (sulfonium ylides and sulfoxonium ylides) are also employed in organic synthesis, e.g. in the Johnson–Corey–Chaykovsky reaction. Another class of ylide compounds is arsenic ylides which are less commonly encountered compared to phosphor and sulphur ylides despite being discovered more than a century ago. However, arsenic ylides have been explored for their synthetic utility and attracted chemist's attention especially as a representative of a different synthesis mechanism compared to phosphorus ylides like Cyclopropanation reaction. The ylide bond plays a key role in all these applications. Despite all these applications, the nature of the ylide bond is still unclear and under debate. [3,4]

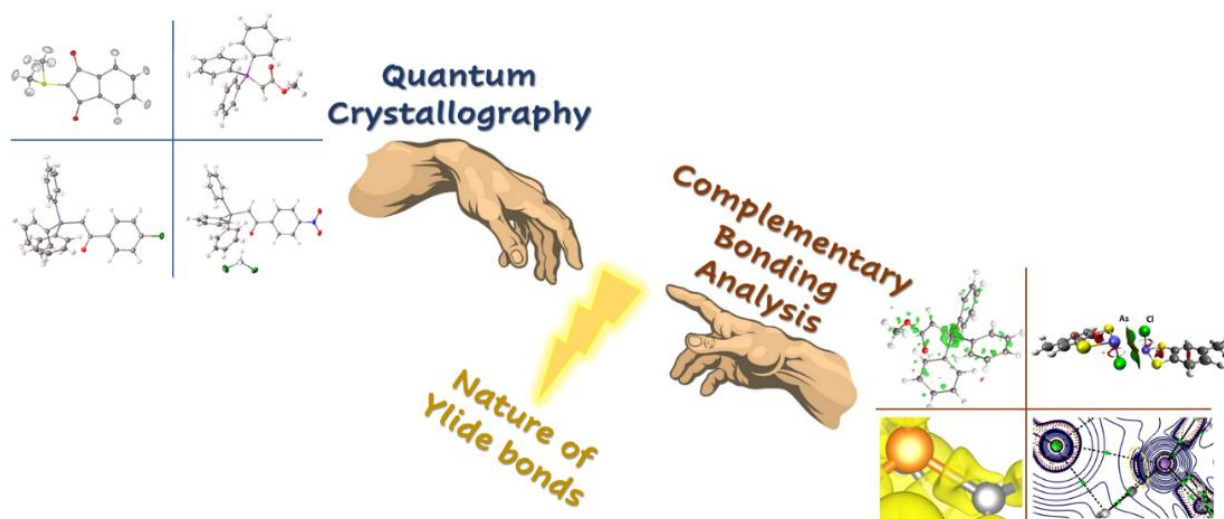


Figure 1. Schematic representation of the study

In this regard, a combination of quantum crystallography (Hirshfeld atom refinement + x-ray constrained wave function fitting) and complementary bonding analysis [5] (QTAIM, ELI-D, EDA, NBO, VBT) reveals the nature and character of the P-C, S-C, and As-C bonds in ylides in detail. It is of practical importance and will also clarify concepts such as the hypervalency of P, S, and As atoms as well as the interplay between covalency and ionicity of heteroatom bonds. To the best of our knowledge, there are four experimental charge density studies about these bonds using multipole refinement, and there is no Hirshfeld atom refinement (HAR) and X-ray wavefunction (XCW) fitting study about these bonds. [6] Here, high-resolution XRD data is collected for one sulphur ylide, two phosphorus ylides, and two arsenic ylides. Then, X-ray wavefunction refinements (HAR + XCW fitting) plus complementary bonding analyses are performed to evaluate the ylide bonds. Our results demonstrate that the

ylide bond is a charge-separated bond with a localized lone pair on the ylide carbon. This bond is an intermediate between covalent and ionic bond and the concept of double bond should be ruled out. Also, the theory of the hypervalent hetero atom (P, S, As) in ylides can be ruled out due to the minor contribution of d orbitals in the bonding and the low energy of this specific orbital interactions. From the energy perspective, the electrostatic term plays a significant role in stabilizing the bond and it influence the bonding more than covalent interactions.

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Poster

From molecular glass to new polymorphic forms in the API sodium naproxen

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The solid form of an API is usually governing its material properties such as solubility or tableting characteristics. Several strategies have been put into place to improve solubility. Naproxen is a poorly soluble API, but its solubility can be improved by synthesizing the corresponding sodium salt. Another alternative to improve solubility is to stabilize an amorphous state [1], however it has been shown that naproxen is a typical non glass former [2]. For ceramic materials, it has been demonstrated that crystallization from glass can be a successful approach [3] to stabilize new polymorphic forms of technological relevance. In this contribution, we have been applying a similar approach investigating sodium naproxen as an example. When heating up sodium naproxen above its melting point, various phases can be stabilized at room temperature depending on the heat treatment: a new polymorph, or a glass phase. This is in significant contrast to pure naproxen. We show in Fig. 1 the temperature dependence of this glass phase as function of temperature. Upon heating, the initial amorphous state (1) evolves towards a second amorphous state (2) before recrystallizing into previously unreported polymorphic forms of sodium naproxen (regions (3) and (4)). For instance, the crystal structure present in the region (4) can be stabilized at room temperature and varies from the initially reported crystal structure of sodium naproxen [4] only by the orientation of the methoxy group (Fig. 1 b).

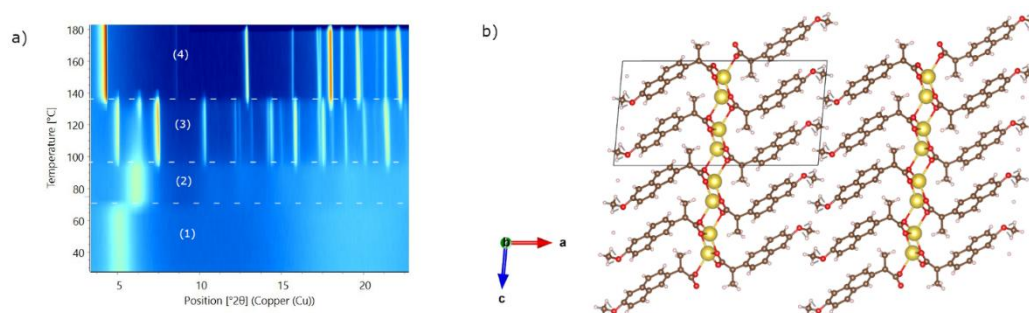


Figure 2: a) Iso-line plot of the recrystallization of amorphous sodium naproxen as function of temperature and b) crystal structure of the new polymorph of sodium naproxen appearing at high temperature (section 4).

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Poster

Intrinsic disorder in MOFs: an untapped resource for materials design

Stefano Canossa

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Latest trends in the chemistry of metal–organic frameworks (MOFs) are seeing non-periodicity under the spotlight, as increasing attention gathers around the concept of short-range order within crystalline networks. Prominent examples include recent efforts towards controlling local sequences of species in so-called multivariate MOFs (1), and structures featuring frustrated flexibility (2). We recently found that disorder is necessary for the construction of MOFs where geometry and connectivity of building blocks are not compatible with an ordered and crystalline structure. Our study focused on the multiphase behaviour of MOFs based on octahedral $Zr_6O_4(OH)_4$ clusters and tetrahedral methane-tetrakis(*p*-biphenyl-carboxylate) linkers. This combination afforded two phases where 12-fold cluster coordination and 4-fold linker coordination are achieved. In both cases, cluster disorder was systematically found as a structural prerequisite (Figure 1), giving rise to distinctive types of aperiodicity such as correlated framework distortion and locally modulated architectures. By combining systematic variation of synthetic conditions and structural analysis by powder and single crystal X-ray total scattering, we revealed intrinsic framework disorder as a largely unexplored degree of freedom for the design of MOF structures with unconventional emergent properties (3).

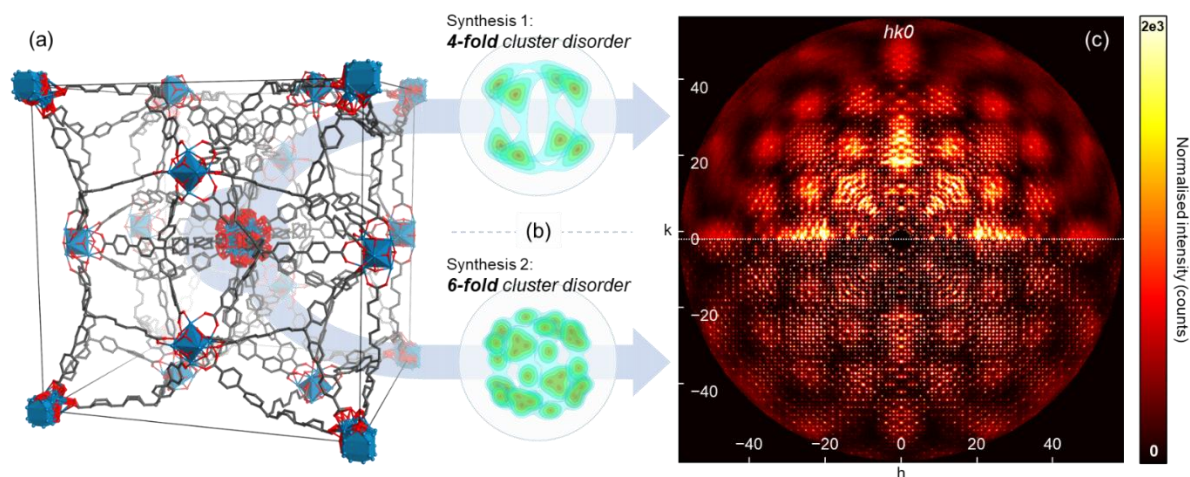


Figure 1. Observed cluster disorder in one of the obtained MOF polymorphs (a), where different local structures generate characteristic electron density maps (b) and single crystal diffuse scattering (c).

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Poster

Self-assembly of sequence-regulated abiotic tetramers for materials mimicking living systems

Elisa Mégroz^{1*}, Konrad Hedderick¹, Sara Kozub², Zihan Li¹, Céline Besnard³, Johanna Brazard¹, Roza Sweda², Takuji Adachi¹

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Biological systems achieved complex self-assembly patterns and sophisticated functionality as a result of evolutionary processes. One of the essential aspects is their ability of synthesizing sequence defined polymers (i.e. proteins) based on 21 canonical amino acids. Although it is possible to make sequence-defined peptides to produce biomimetic materials, the cost and time to prepare them limit their application. Recently, owing to the development of synthetic methods, large scale production of abiotic polymers with defined sequence became possible. This new class of materials has opened an opportunity to achieve complex morphology using abiotic polymers such as polycarbamates and polypeptoids. We initiated the investigation to understand how the sequence of an abiotic polymer affects the morphology through the regulation of inter- and intramolecular interactions. In this study, carbamate (RO-CO-NHR') was chosen for the monomer backbone because of its similarity to peptides (R-CO-NHR'). Instead of polycarbamates, tetramer was used as a simpler model system to build a foundation (Fig. 1A). Four sequences with varied order of chirality were studied: Boc-SSSS, Boc-SSSR, Boc-SRSS and Boc-SRSR.

Due to limited solubility of the compounds in solvents, we prepared a film through melt and cool process. Freshly prepared samples are typically featureless amorphous film. However, we realized that the morphology of films continued evolving over days. It was identified that moisture plays a critical role, and therefore films were annealed by water vapor to accelerate the morphological

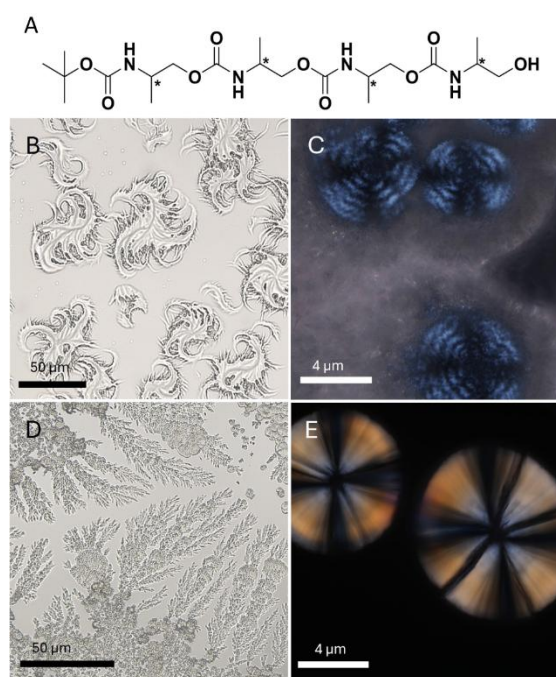


Figure 3 (A) chemical structure of the tetramer, (B) amorphous spiral and (C) twisted spherulite of Boc-SRSS, (D) amorphous region and (E) spherulite of Boc-RRRR

evolution. Surprisingly, morphological patterns that are reminiscent to what can be found in nature appeared (Fig. 1B and D). These patterns eventually convert to spherulites (Fig. 1C and E). The details of films were characterized using Raman microspectroscopy, optical microscopy while crystal structures were obtained by using microED. In three sequences, polymorphs were observed.

Clear differences were observed in the film morphology between four sequences (Fig. 1B-E). Raman spectra support that the sequences alter the intermolecular hydrogen bonding patterns. Among them, Boc-SRSS shows particularly fascinating morphology including amorphous spiral phase and twisted spherulites (Fig. 1B and C).

At the presentation, a peculiar role of water for self-assembly process, morphological differences between sequences, and crystallization pathways involving morphologically sophisticated amorphous phase will be discussed.

Poster

Salen-derived heterometallic complexes

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Salen is one of the most studied ligands in chemistry, notably for its straightforward synthesis and its ability to coordinate to a variety of metal ions.^[1] This Schiff base compound has a N_2O_2 chelate site allowing the coordination of one metal ion. Salen is a versatile ligand that can be functionalized to create a wide range of new ligand structures, offering numerous possibilities for further functionalization.

In our studies, we aim at synthesizing heterometallic complexes with two or three different metal ions. To achieve this goal, salen can be functionalized with glycol chains creating e.g. a O_3O_3 recognition site for a second metal ion. The combination of different metal ions can provide enhanced chemical and biological properties.^[2] For instance, the synthesized heterometallic complexes could be used as mixed metal oxide precursors or show potential synergic antibacterial properties.^[3] In addition, functionalized salen with aromatic rings (e.g. naphthalene) can be used as fluorescent sensor.^[4] We report the results for several antimicrobial tests, mixed metal oxide precursors, and fluorimetric sensing.

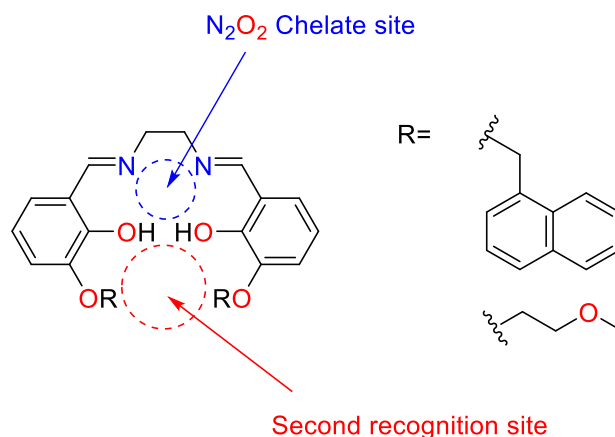


Fig. 1 : Representation of salen-derived ligand with N_2O_2 chelate and second recognition sites.

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Poster

Revisiting the crystal structure and magnetic properties of $M(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ ($M = \text{Ni}^{2+}, \text{Co}^{2+}$) compounds – A combined theoretical and experimental approach

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In modern technology, ferro-, ferri- and antiferromagnets show a potential to replace conventional electronics and energy materials in a variety of applications [1]. In the last years, transition metal phosphates are receiving growing attention owing to their peculiar magnetic properties [2,3].

In this study, we focus on transition-metal intercalated vanadyl-phosphates. In literature, $M(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ ($M = \text{Ni}^{2+}, \text{Co}^{2+}$) compounds are described as tetragonal, space group I/mmm . The structure consists of layers of a 4-connected net where corner-sharing VO_5 and PO_4 tetrahedra alternate. Water molecules in form of aquo-ligands and octahedrally coordinated transition metal cations sit in-between the VOPO_4 layers [4] (Figure 1a). These materials were interpreted as having a bulk ferromagnetic coupling, due to the existence of $\text{V}=\text{O}-\text{M}-\text{O}=\text{V}$ linear trimers and the corresponding nearest neighbor $\text{V}^{4+}-\text{M}^{2+}$ interactions within them. Possible intralayer antiferromagnetic interactions have been described as weak and insignificant [5].

By implementing relevant modifications to the known synthesis routes, which were lacking in detail for certain steps, we successfully obtained single crystals of the title compounds. Our structural investigations indicated a tetragonal symmetry, but a lower space group ($I4/m$) with respect to previous studies. New magnetic susceptibility measurements were also conducted. The applied magnetic field was oriented parallel and perpendicular to the c-axis. In contrast to literature data, our results indicate the presence of a low-dimensional magnetic system. Furthermore, we observe a different temperature dependence of the molar magnetic susceptibility for the two orthogonal field directions, as well as different value ranges for the two compounds. Larger values of χ_m were observed for the Co-compound in comparison to the Ni-Compound, implying a difference in the bulk magnetic behavior. Compelling evidence implies that there are competing antiferromagnetic and ferromagnetic interactions in a system of a presumed 2D connectivity, where the former ones could have a much more substantial role.

To interpret the magnetism in terms of structure-property correlations, preliminary calculations by DFT+U methods, as implemented in the *CP2K* code [6,7] are currently in progress in order to obtain the electronic structure, orbital population density and theoretical magnetic properties.

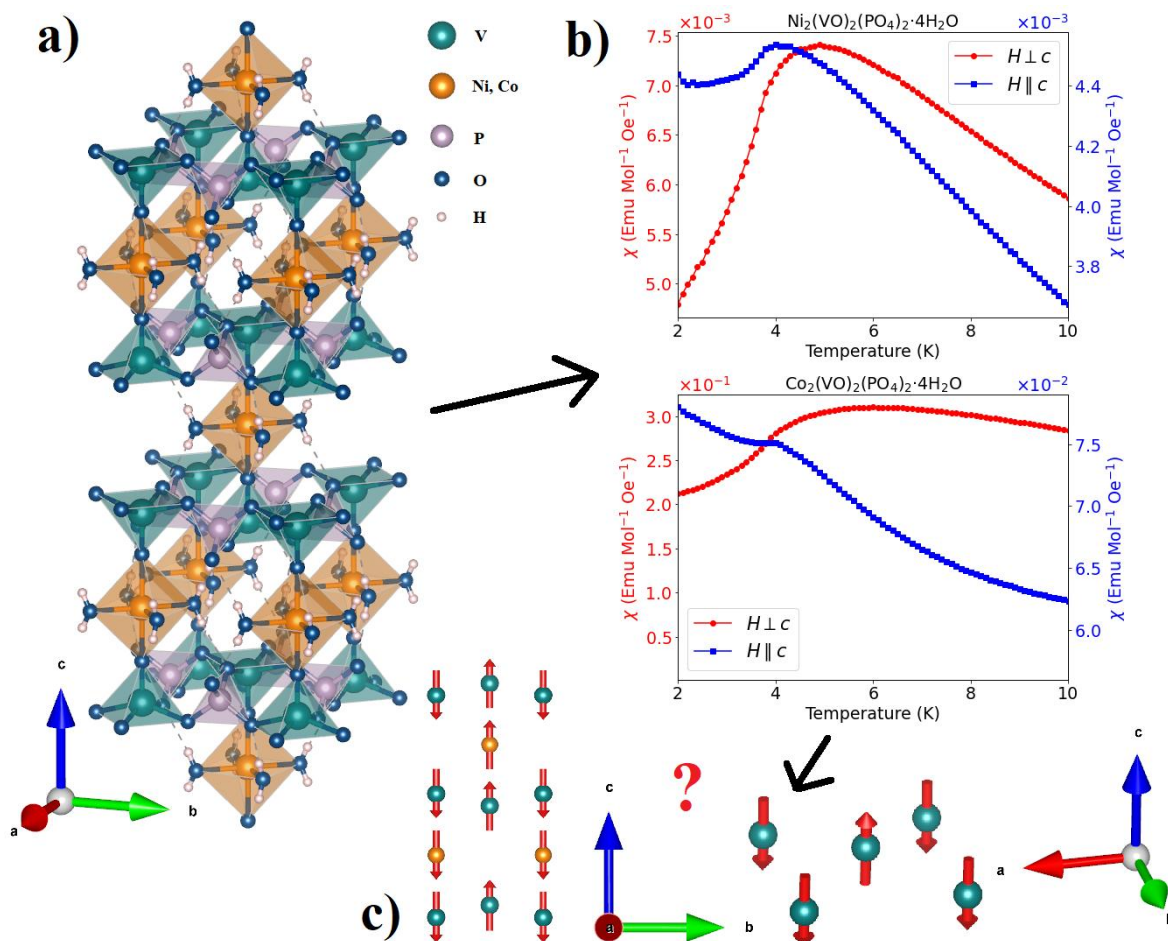


Figure 4 - a) Crystal Structure of $M(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ ($M = \text{Ni}^{2+}, \text{Co}^{2+}$) compounds b) Molar magnetic susceptibility of the respective $M(\text{VO})_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ compounds measured in different orientations c) Plausible magnetic structure of the title compounds

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Poster

A score and nine years of irbesartan

Philippe Ochsenbein*, Michel Bonin, Farzaneh Fadaei-Tirani, Marie-Hélène Lemée, Jérôme Kieffer,
Daniel Görl, Mohamed El-Hajji and Kurt Schenk-Joß*

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Abstract

Irbesartan is a non-peptide antagonist of the angiotensin-II-AT1 receptor and is used for the treatment of hypertension. Here, the history, achievements and open questions related to irbesartan are examined. Tautomerism of the tetrazole moiety leads to two desmotropes, A and B. Roughly ten dozen data collections on single crystals at various temperatures, from X-rays and neutrons, are presented, deposited and interpreted; new structures are described and a detailed evolution of the thermal expansion is achieved. Disorder of the *n*-butyl-chains is observed in A and B. The trigonal desmotrope A builds its structure incorporating a hydrate channel upon nucleation. The hydrophobic nature of the *n*-butyl-chains induces the growth of a flat crown of chains in a meta-stable phase, disappearing after the thermally activated creation of a *gauche* conformer that distorts this wreath to a more prolate shape. This irreversible, conformational transition leads, henceforth, to a different evolution of lattice parameters and thermal expansion; the water inclusion explains the strained, imperfect crystallites, complex solubilities, a capricious packing coefficient and slow growth. In the triclinic desmotrope B, the all-*trans* → *gauche* disorder in the *n*-butyl-chain leads to random, diffuse changes in the structure between 265 and 165 K. As confirmed by calorimetry and thermal expansion, these subtle, local re-arrangements do not affect the space group and trigger a reversible, first-order phase transition at 208 K. The neutron study brings desirable clarity regarding the geometry of the tetrazole and its hydrogen, and precious reference values for the weak interactions. Focussing on the tetrazole and the *n*-butyl-chains, we propose an alternative interpretation of the ¹⁵N NMR spectra, published more than two decades earlier.

Poster

An *ad hoc* Absorption Correction for Reliable Pair-Distribution Functions from Low Energy x-ray Sources

Till Schertenleib, Yucong Chen, Andrew Yang, Daniel Schmuckler, Geng Bang Jin, Pascal Schouwink, Wendy L. Queen, Simon J.L. Billinge

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In this work, we explored data acquisition protocols and improved data reduction protocols using PDFgetX3 to obtain reliable data for atomic pair distribution function (PDF) analysis from a laboratory-based Mo K α x-ray source. A variable counting scheme is described that preferentially counts in the high-angle region of the diffraction pattern. The effects on the resulting PDF are studied by varying the overall count time, the use of Soller slits, and limiting the out-of-plane divergence of the incident beam.¹

In contrast to synchrotron experiments, we demonstrate how sample absorption effects can no longer be ignored in lab-based diffractometers. We present an analytical and *ad hoc* solution based on statistical methods that can correct for those absorption effects and results in more reliable PDFs from lab-based instruments. The correction was put to test on a set of materials with varying attenuation coefficients that were measured using laboratory-based Mo and synchrotron x-rays. We provide an easy-to-use software that applies absorption corrections to diffraction data with minimal user input and provide a Python script that allows a quantitative comparison of PDFs obtained from different sources.²

References

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- (2) Y. Chen, T. Schertenleib, A. Yang, P. Schouwink, W. L. Queen, S. J. L. Billinge. An *ad hoc* Absorption Correction for Reliable Pair-Distribution Functions from Low Energy x-ray Sources. (manuscript under preparation)

Poster

Exploring High-Throughput Synchrotron X-ray Powder Diffraction

R.N. Widmer¹, R. Pokratath¹, M. Reinle-Schmitt¹, T. Stoll¹, F. Gozzo*¹

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Industrial X-Ray powder diffraction measurements conducted at synchrotron facilities (S-XRPD) are at present primarily used for research & development and advanced troubleshooting. This is due to the operational complexity, limited accessibility, and higher costs associated with synchrotron measurements compared to laboratory instrumentation. High-throughput systems can bridge this gap between traditional laboratory instrumentation and conventional synchrotron measurements¹. Importantly, the concept of high-throughput measurements not only entails accelerated and automated data collection, but also streamlined sample preparation and efficient data analysis, thereby reducing overall costs. In this presentation, we explore applications of high-throughput S-XRPD for the characterization of pharmaceuticals.

We assess the performance of a novel high-throughput S-XRPD system against several relevant experimental parameters based on a systematic evaluation of the resulting data quality. This includes signal-to-noise ratios as a function of collection time, reproducibility of peak intensities, reliability of quantification of known mixtures, and achievable level of detection. To this end, we investigate a range of experimental parameters across a set of pharmaceutical powders with typical physical properties. Our analysis aims to carefully assess the balance between the obvious advantages of streamlined experimental logistics and the data quality, compared to standard capillary measurements. Sample preparation times under one minute per sample, automated measurement of up to 50 samples per batch, digital tracking of sample IDs based on DMC codes, and efficient data analysis protocols enable scalable and cost-effective handling of industrial projects.

Based on preliminary results, we envision a variety of applications that will significantly benefit from synchrotron radiation but do not demand ultimate levels of detection or peak shape quality. This promising middle-ground of efficiency vs. quality bridges industrial requirements with state-of-the-art synchrotron-based measurements. Furthermore, the additional benefit of fast and easy sample preparation in relatively large batches makes it possible to comply with industrial requirements for in-house sample preparation. Preliminary results to assess the performance of the system beyond the mere qualitative routine analysis will also be discussed, which is integral part of our on-going developments.

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*Corresponding author: fabia.gozzo@excelsus2s.com

Poster

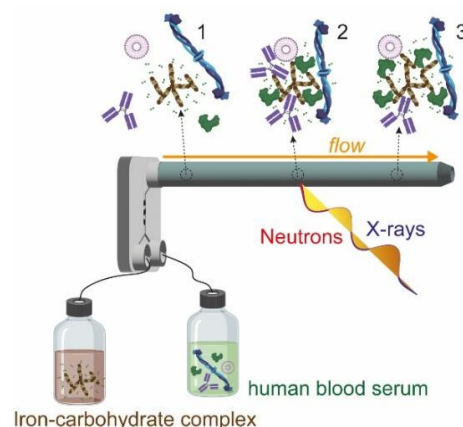
Iron-carbohydrate complexes for anaemia treatment: understanding the dynamic interactions with human blood serum

Leonard Krupnik^{1,2,3}, Jonathan Avaro^{1,4}, Bruno Silva^{1,4,5}, Reinaldo Digigow⁶, Amy Alston⁶, Erik Philipp⁶, Beat Flühmann⁶, Peter Wick³, Antonia Neels^{1,2}

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5.Laboratory for Biointerfaces, Empa, St. Gallen, Switzerland. 6. CSL Vifor, Glattbrugg, Schweiz.

Intravenous (IV) iron-carbohydrate complexes (ICCs) are widely used nanoparticles (NPs) to treat iron deficiency anaemia, associated with chronic kidney disease, cancer and other etiologies (1). However, despite the abundance of physicochemical characterisation data and clinical studies for these formulations, clear evidence-based understanding linking the physicochemical properties of ICCs with their clinical outcome remains elusive (1). Studies suggest that early interactions between NPs and blood upon IV injection are key to understanding how differences in physicochemical characteristics of ICCs exhibit different structure-function relationships (2). We therefore investigated the nano-structure of two clinically applied ICCs, iron sucrose (IS) and ferric carboxymaltose (FCM) (3) using small-angle X-ray and neutron scattering (SAXS/SANS). We revealed important differences in the surface morphology of these two ICCs, as FCM showed a localised carbohydrate shell, in contrast to IS, which showed a diffuse layer of carbohydrate ligand. We hypothesised that such differences in carbohydrate morphology influence interactions with blood, which motivated us to study the dynamic interactions between ICCs and human blood serum under flow using microfluidic SAXS/SANS (Fig. 1). We found that the interactions between FCM and human blood serum are different compared to IS and additionally depend on flow and NP concentration. Our approach sets a path for detailed investigations of the correlation between physicochemical properties of iron-carbohydrate complexes, their structure-function relationships, and ultimately clinical outcomes.



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BUSINESS USE

SGK/SSCr: General Assembly 2024

SGK/SSCr – Basel, Innovation Park, 12.09.2024



Swiss Society for Crystallography SGK/SSCr General Assembly 2024

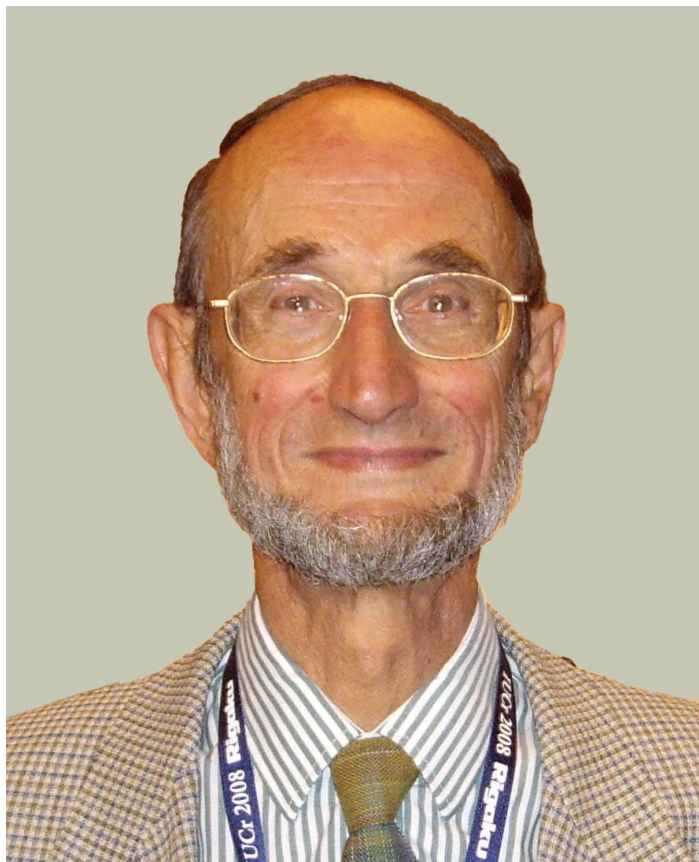
Thursday, 12.09.2024, 12:40-13:30
Switzerland Innovation Park Basel Area AG, 4123 Allschwil

Agenda:

- 1) Determination of the quorum according to Art. 12/by-laws
- 2) Proposition for acceptance of the minutes of the General Assembly 2023, Zürich
- 3) Proposition for changes in the bylaws
- 4) Reports
 - a) Annual report
 - b) New incentives
 - c) Delegates to adhering bodies (IUCr, ECA, IOCG)
 - d) Annual financial statement
 - e) Budget for next year
- 5) Elections
 - a) Definition of a chairperson for the elections
 - b) Confirmation of the present board members
 - c) Change of presidency, proposition Simon Grabowsky (Bern)
 - d) Nomination of new board members. To be submitted to the president 10 days prior to the general assembly.
 - e) Confirmation of SCNAT delegate
 - f) Election/confirmation of the auditors
- 6) 2025 Meeting and General Assembly. Decision on location and organizer (EPFL, Lausanne, Arnaud Magrez and Pascal Schouwink). Proposals for 2026 are welcome!
- 7) Other motions of members and communications (please communicate to the president 10 days prior to the meeting)

The minutes of the last General Assembly (University of Zürich, Friday, 08.09.2023, 13:15 – 14:15) are published [on page 49-55](#) of the present issue SGK/SSCr newsletter N112, August.

Obituary: Dieter Schwarzenbach 1936-2024



Dieter passed away in Lausanne at the hospital after a long neuro-degenerative decline. He is leaving behind his wife Vera and his two children Charlotte and Thomas.

I met Dieter in 1966 when I started my doctoral studies at the Institute of Crystallography at the ETH in Zurich. That was shortly before his departure for a postdoctoral internship in the United States. In 1969 he returned to Zürich bringing with him the newly developed X-ray System of programs for the solutions of crystal structures. I was very fortunate to take advantage of it: it allowed me to crack a difficult structure by direct methods and finalize my PhD thesis. Later, it was also Dieter who helped me find the most suitable place for a postdoctoral position in

David Templeton's group in the Lawrence Berkeley laboratory.

The American experiences gained by Dieter first in Pittsburgh in Prof. George Allen Jeffery's Department of Crystallography and then in UCLA in Prof. Ken Trueblood's Laboratory in addition to his PhD with Prof. Fritz Laves' group at the ETH in Zürich was an excellent prerequisite for a successful career in crystallography. Indeed, shortly after his return from the US, he was offered in 1970 a position as a lecturer in the Science Faculty at the University of Lausanne for a basic course in Crystallography. Three years later, he was offered to create and lead the Institute of Crystallography in the same institution with a position of extraordinary professor which was later promoted to full professor in 1978.

My stay in Berkeley was coming to an end when Dieter visited me in 1973 and invited me to complete his team in Lausanne. Thus in 1974, I returned back to Lausanne to pursue my career in crystallography as a lecturer in Dieter's lab.

Since its creation, the Institute of Crystallography delivered lectures and practical courses in various fields of crystallography to students at the University of Lausanne (UNIL) and of the Federal School of Technology (EPFL). In particular, students of physics, chemistry, materials and earth sciences followed the basic and advanced courses. Our common book (Cristallographie, EPFL-Press, Lausanne (2006)) resulted from our experiences in teaching crystallography.

In parallel, the research of Dieter and his team developed in numerous directions of crystallography. The field of electron density by diffraction method in crystalline structures was an important aspect of Dieter's interests. Would precise electron densities measured by diffraction be able to reproduce some physical quantities like e.g. electric field gradients (EFG)? One of his most cited articles (Acta Cryst. (1982). A38, 733-739) concerned the charge densities and EFG in Corundum $\alpha\text{-Al}_2\text{O}_3$ where the capabilities and limits of the diffraction methods were clearly demonstrated. Other important studies followed namely charge densities in cuprite, Cu_2O (Acta Cryst. (1986). B42, 201-208) published with his PhD student Renzo Restori where the influences of the data reduction processes, anisotropic displacements and the deformation models were

explored. Other compounds like Li_3N , TiO_2 , CoS_2 , NiS_2 were all part of an important study program on charge densities.

During his career, Dieter developed some very fruitful collaborations with other colleagues from nearby institutions. Hans-Beat Bürgi, head of the Laboratory of Crystallography in Bern and Howard Flack from the University of Geneva were among them. The recent discovery of C60 were the subject of many interesting studies both in Bern and Lausanne. The software development of the XTAL system of programs by Dieter's PhD student Eric Blanc, greatly contributed to the successful results. His LSLS program (for Lausanne least-squares module) had some new capabilities on absorption, extinction corrections and twinning which led to the C60 publication in *Angewandte Chemie International* (1992), 31/5, 640-643). This fruitful collaboration on fullerenes resulted in four additional papers on various modifications and phases, improving models and obtaining more precise data on the orientational disorder and C-C atomic distances.

Dieter and Howard Flack published an important series of well cited publications related to some new theoretical developments in the methodologies of crystal diffraction. Both laboratories were involved in the software developments of the XRAY system and its successor XTAL. About a dozen of publications covering various topics from the use of least-squares restraints for origin fixing in polar space-groups (Acta Cryst. (1988), A44, 499-506) to the evaluation of transmission factors and their first

derivatives with respect to crystal shape parameters (J. Appl. Cryst. (1991), 24, 1035-1041) were published. Perhaps the most tangible result of their collaboration was the establishment of the Subcommittee on Statistical Descriptors by the International Union of Crystallography (IUCr). A panel of international specialists in statistical methods in physics and crystallography joined their efforts to establish a series of recommendations for the proper treatment of statistical errors in crystallographic research. Dieter was the chair of the panel which also included Howard as a member. The two reports on Statistical Descriptors in Crystallography I and II appeared in Acta Cryst. (1989). A45, 63-75 and Acta Cryst. (1995). A51, 565-569. They listed a series of 13 recommendations, the validity of which form the basis of current statistical treatment of crystallographic data. It is owing to the second report that the usual concept of e.s.d. (estimated standard deviations) were replaced by the more accurate term "standard uncertainties" (s. u.).

By studying the impressive list of Dieter's scientific publications, close to 150, I was struck by the diversity of his interests which covered a very large number of fields in crystallography. They extended from historical notices to mathematical crystallography, symmetry, diffraction theories and structure modeling to cite only the most important topics. Dieter had an excellent memory and he always impressed his audience with his vast knowledge of crystallography.

Dieter has always been active in the Swiss and international crystallographer's activities. He was

president of the Swiss Crystallography Society from 1984 to 1987. It was under his chairmanship and with the professional support of the Society's secretary, Howard Flack, that the bulletin of the Swiss Society was established. Earlier, the team formed by Walter Petter and Dieter Schwarzenbach led to the very successful organization of the ECM-3 conference on the ETHZ Höggerberg's site which took place in September 1976. The buildings were just inaugurated and the international participants were especially impressed by the quality and luxury of the new facilities and especially the marble decorations. On the international level, Dieter was co-editor of Acta Cryst. A and B from 1992 to 1999 and immediately after he was appointed Section Editor of Acta Cryst. A until 2011.

Under the leadership of Dieter, the Lausanne Institute of crystallography attracted a large number of international visitors. This was facilitated owing to two institutions found in Lausanne, namely the Herbette Foundation from UNIL and the "3e cycle" of physics (which would now be called a doctoral school) of the French-speaking part of Switzerland. Both institutions were able to support the visit of international lecturers for a few months. During that period, we could greatly benefit from the lectures of a very impressive panel of specialists including among them Aloysio Janner, Ted Janssen, David Templeton, Pierre Toledano, Richard Wellberry, Terry Willis, Hans Wondratchek and Akiji Yamamoto. The first version of Richard Wellberry's book on X-Ray Diffuse Scattering appeared in Lausanne as lecture notes on the

same subject! It was also in Lausanne that Howard Flack developed his concept about his famous parameter during the visit of David Templeton and the fruitful discussions on Rodger's η parameter.

Under Dieter's direction the Institute of Crystallography led to the creation of the very successful Swiss Norwegian beamline (SNBL) at the ESRF in Grenoble. In the beginning, the essential problem for Dieter and Hans-Beat Bürgi (who was also interested in this facility) was not the financing of the beamline but rather to find first common objectives between the two participating countries and create common visions to lead the project. It took a few years to solve all the administrative problems leading to the creation of the SNBL Foundation. Today the SNBL is a flourishing institution for the benefit of the Swiss and Norwegian scientists.

Dieter most admired characteristics among the institute members was his deep knowledge of the history of Switzerland. He could also cite entire poems of the German and English literature, in particular extracts from Goethe's Faust and quotes from Shakespeare.

Dieter was a fine musician and a very sportive person. His career as a musician already started as a student in 1957 as a violinist in the Zurich Academic Orchestra. He pursued his musical activities in Lausanne long after his retirement and participated actively in a few amateur orchestras, very often along with Vera who is also an appreciated violist. Dieter was also very

sportive and not afraid to ride his bicycle every day for about 12 km to travel to the Institute of Crystallography and back home with a non-negligible height difference. He appreciated to ride his bicycle accompanied by his son and did not refrain sometimes traveling for more than 170 km to make a tour around the lake of Geneva. He was also a real mountaineer and randonnée skier. I had many opportunities to climb with him several Swiss summits both in summer and winter. I remember very clearly our party of four starting from Rothenboden over Zermatt for the ascent of the Pointe Dufour, the highest point in Switzerland (4'634 m) by ski touring. Finally, toward the end of the ascension, only the two crystallographers managed to reach the summit.

Dieter also joined from the very beginning the basketball team called OURRS bringing together professors from UNIL and EPFL. Every Tuesday, we meet together during the semester for an hour of physical exercise and basketball game. Dieter participated actively in the team activities until his physical abilities started to diminish. Unfortunately, Dieter passed away just a few days before the celebration of the 50th anniversary of the team.

A slightly modified version of this article will appear in Acta Cryst. A80.

The help of Vera Schwarzenbach, Alla Arakcheeva, Eric Blanc and Pascal Schouwink is acknowledged for providing useful information in writing this article.

By Gervais Chapuis

Lausanne, August 2024

Report on the Zürich School of Crystallography

By Hans-Beat Bürgi, Tony Linden, School Directors

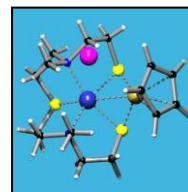
The Zürich School of Crystallography

Bring Your Own Crystals



University of Zürich

June 17 - 29, 2024



The 11th Zürich School of Crystallography was held as usual in the Department of Chemistry at the University of Zürich (UZH). The 10 male and 10 female participants comprised one MSc and 13 PhD students, 3 postdocs, 2 research staff and one person from a pharmaceutical company. They came from 17 countries: Brazil, China (Hong Kong), Croatia, Denmark, France, Germany, Italy, Japan, Norway, Saudia Arabia, Singapore, Slovenia, Sweden, Switzerland, Tunisia, USA and Zimbabwe. The cohort included 11 full-time tutors and two local guest lecturers.

All of the participants were highly dedicated and worked tirelessly for the entire School, despite its intensity. While most participants were young scientists, the group this time included two upcoming service crystallographers. The levels of experience of the participants ranged from minimal to moderate experience. During casual interactions, we gained the clear impression that everyone felt happy that they had learnt something new and were more confident about tackling their own structure determinations.

Participants receive very personalised mentoring with our popular 2:1 student-tutor ratio and are additionally

motivated by the "bring-your-own-crystals" concept of the school. They become well-equipped to determine their own structures when they return home and to recognise when they need to seek advice for a challenging problem. One participant was thrilled that the information on growing crystals, sent out before the School, had yielded instant results for the materials she had hitherto been struggling to crystallise. Many new friendships formed and it was pleasing to see everyone interacting with each other.

The aim of the School is to introduce the participants to the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination. We cover all stages from crystal growth through to interpretation of the results and preparing material for publication. We deliberately limit the focus to single-crystal small-molecule crystallography so as to be thorough. The daily schedule combines a balance of lectures, tutorial exercises and practical work, including hands-on experience mounting crystals and collecting data from samples the participants provide. We use five diffractometers, which include dual-source Rigaku Synergy and Supernova instruments, as well as a Bruker Venture D8 diffractometer.

The concepts of symmetry are consistently a challenging theme, which



appears in part to be related to the visualisation of objects and symmetry transformations in 3D. Online tools are useful, but are not truly 3D. In small tutorial groups, we use wooden and plastic

models of solid shapes and molecules representing all point groups. The ability to hold and tumble such models helps the participants acquire the concepts more easily. It was also great fun watching people cutting their apples in the "La coupe du roi" exercise to illustrate stereochemistry and chirality, a demonstration initially presented during our schools by Howard Flack.

An innovation introduced this time by Lukas Palatinus was the use of short quizzes via the Kahoot platform. A multiple-choice question is beamed on the front screen and participants have a limited time (e.g. 30 seconds) to answer the question using their phones. The results are then displayed on the front screen, which allows quick discussion of the answers and clarification of any

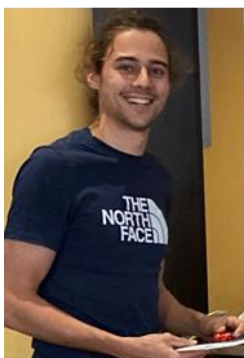


misunderstandings. Points are awarded for correct answers in the fastest time. The quizzes generated excitement and enthusiasm, while providing instant feedback and reinforcement of key points from the preceding lecture material.

During the practical component, the participants work on at least four example structures presenting varying degrees of difficulty. This facilitates learning how to use effectively the software and to handle frequently encountered challenges, such as entities lying on or across symmetry elements, disorder, absolute structure and the analysis of weak interactions. Participants learn about the actual procedures going on when various buttons and settings are selected in the software and to interpret whether or not

software. The extensive range of tools and graphics incorporated into Olex2, from routine tasks like atom-naming to modelling disorder, plus a range of quality indicators and statistics, allows us to demonstrate structure solution, refinement and results evaluation in a didactically beneficial way.

Most days concluded with a short discussion where participants can express their feelings about their experience that day. On the final morning, the participants sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge. After the exam, the final day included some advanced topics and presentations designed to give the participants a taste of other possibilities, such as Hirshfeld atom refinements and electron diffraction.



appropriate results are obtained. Each participant then works on the data set collected from their own crystalline sample. We used Olex2 once again, alongside the SHELX programs, PLATON and other readily available

The farewell banquet is an emotional time for everyone after making so many new friends. Each participant received a certificate, Swiss chocolate and a copy of The Non-Ambient Guide donated by Anton Paar. The two participants with

the best exam results received additional prizes: an insulated UZH-branded coffee mug (1st) and the old but still useful book *Crystal Structure Refinement, A Crystallographer's Guide to SHELXL* by Peter Müller (1st & 2nd).

The personal impressions of two participants are given below. We anticipate organising the next School in June 2026.

We gratefully acknowledge the generosity of our sponsors and supporters: Department of Chemistry of the University of Zürich, Swiss Society for Crystallography, European Crystallographic Association, International Union of Crystallography, Cambridge Crystallographic Data Centre, Rigaku Oxford Diffraction, Dectris Ltd, Bruker AXS, Anton Paar and Quantum Detectors.

The Zürich School of Crystallography 2024 – impressions from participants



***Voon Kunn Ng,
National University
of Singapore***

My experience during The Zurich School of Crystallography 2024 was a truly rewarding one. Not only did I gain theoretical and practical knowledge on Crystallography, the interaction with tutors and participants has also introduced me to various cultures, forged friendships and created many fond memories.

The School was very well-organised, and students were very well taken care of. Even before the School started, we received the lecture notes and many

reading materials to prepare us for the School. Detailed instructions on downloading the software were also provided in advance, giving us ample time to resolve any software issues. Tutors even made time to solve any software issues on the first day, ensuring that all of us were well-equipped when classes started the next day.

While instrument operation and data processing are not new to me, I was curious to understand what the significance behind every step was. In this aspect, the School did not disappoint and provided answers to my questions. There was still so much that I could learn despite having solved many structures myself. Small group tutorials were especially helpful to visualize space groups and symmetry operations, and tutors were very approachable to answer any queries that we had. I could feel the passion and enthusiasm that the tutors had for Crystallography as they were teaching and explaining, making it extremely pleasant to learn from them.

Classes were highly intensive and coffee breaks to take a breather were very much looked forward to. The free day in the middle of the School also provided some rest time and an opportunity to explore the city. Even though ten days of Crystallography was exhausting, knowing how much effort the tutors put in made me determined to absorb the knowledge that they were passing on.

On the last day of classes, all students sat for a 2-hour examination to test our knowledge gained during the School. As someone who last sat for an exam many years ago, it was nerve wracking,

yet I was eager to know how much information I had acquired in the past ten days.

To sum it up, the School has taught me to greatly appreciate Crystallography. It was an engaging and enriching experience, getting to know people in the field and learning so much from them. I would like to thank the organisers, Professor Tony Linden and Professor Hans-Beat Bürgi, for the opportunity to participate in the School, and making sure that we were always getting the best out of it.



**Andrea Vitale,
Bologna, Italy**

During the second half of June, from the 17th to the 29th, I had the opportunity to spend time with 19 other young researchers from all over the world in Zurich, Switzerland, for the Zurich School of Crystallography 2024.

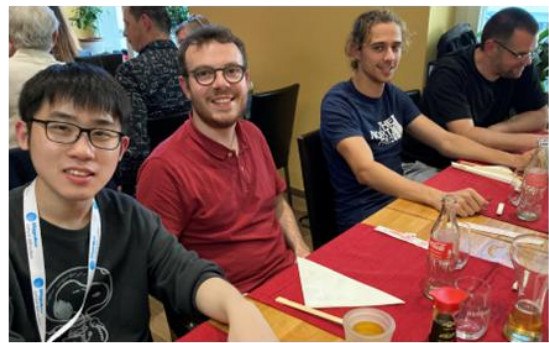
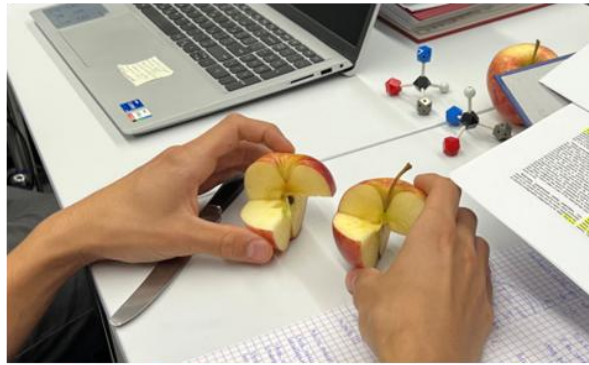
It was a beautiful and formative experience, offering one of the most comprehensive understandings of crystallography and its related fields, both in practical applications and research.

Professors Anthony Linden and Hans-Beat Bürgi organized and directed the school in an exceptional manner. From the incredible selection of well-prepared tutors, who guided us through this intense and educational journey, to the carefully chosen hotel and restaurants that facilitated socializing and provided opportunities to meet and converse with professors and fellow researchers sharing the same passion. These interactions were inspiring, offering

various perspectives and topics in this field.

For me, the school greatly enhanced my understanding of the foundational aspects of my research, particularly concerning the theory behind structure solution and refinement models. Every lecture was filled with information, tips, and tricks that crystallographers can use in their daily work. All this magnitude of knowledge was provided in both paper and .pdf formats, which will be very useful for continuing my studies and supporting my research projects. Additionally, we had the chance to collect diffraction intensities from our own crystals using the most advanced diffractometers and detectors for single-crystal structure determination. This hands-on experience allowed me to learn more about the instruments and their software, and it gave me the opportunity to solve and refine my own synthesized structure, manage its disorder, and study its packing within the unit cell.

In conclusion, the Zurich School of Crystallography has been the highlight of my first year in my PhD program. It has already significantly contributed to my future career, research, and experiments, and it provided the chance to meet incredible people whom I look forward to encountering again in the future.



Report on the Erice Crystallography School 2024

By Dubravka Sisak Jung

The 59th Course of the International School of Crystallography "Powder Diffraction: Advancing Real Materials in the Information Era," took place from May 31 to June 8, 2024, directed by Dave Billing, Matteo Leoni and Dubravka Sisak Jung. The event gathered top scientists, researchers, and students from around the world to explore the latest developments in crystallography at the Ettore Majorana Foundation and Centre for Scientific Culture in Erice, Italy.

In the history of International School of Crystallography, this was the second course dedicated to powder diffraction, following the course on Power of Powder Diffraction, held in 2011.

This year's course gathered 83 students, 28 lecturers and workshop tutors, and 9 meeting organizers. Lecturers included 20 men and 8 women, coming from 12 countries. Worthwhile mentioning is that many of the lecturers were affiliated to the first powder diffraction school, either as directors, lecturers or student. Participants included 33 women and 50 men, coming from 28 countries in Europe, Asia, North and South America, and Africa. Participants were largely PhD students, postdocs and young researchers, with some participants from industry. Swiss Society for Crystallography (SSCr) was well represented in the School. Dubravka Sisak Jung (member of the board) was one of the three scientific directors. Furthermore, four lecturers were affiliated with the SSCr: Paula SGK / SSCr Newsletter No. 112 (2024)

Abdala and Nicola Casati (members of the board), and Lynne McCusker and Fabia Gozzo (members). Three participants of the School are also affiliated as SSCr members.

The program was designed to provide an overview of a wide range of topics and encourage participants towards further learning. The daily schedule included either lectures or workshops in the morning, followed by lectures in the afternoon.

The sequence of lectures was scheduled to start with some of basic concepts of powder diffraction and scattering and to progress to more contemporary methods (hybrid and tandem techniques, computational methods, machine learning).

The school offered 12 workshops, aiming to introduce participants to software packages and their practical use. Even if a hands-on tutorial was not always possible, the students were provided with extensive documentation and some step-by-step instructions to continue the learning independently after the school. Two topical workshops included Python programming basics and the use of Python for machine learning in crystallography and powder diffraction. These can be considered a first of their kind in a crystallography school, and they provided soft skills likely to prove invaluable in the future.

Two evening poster sessions allowed participants opportunities to present



Celebration of the 50th (golden) anniversary of the International School of Crystallography with golden glasses.

and engage with delegates on their research. With posters displayed over two sessions, the event facilitated vibrant discussions and excellent networking opportunities.

The course included two panel discussions. The panel on metadata and data aimed to raise awareness of importance of producing meaningful, correct and standardized powder diffraction data. The panelists included beamline scientists, industry

professionals and university professors. The panel “Young crystallographers ask” aimed for an open discussion between participants and lecturers on science and careers in crystallography.

Awards and participants’ feedback

During the closing ceremony, awards were presented to the best posters, recognizing outstanding contributions: Marta Morana (University of Florence, Italy), Anna Mauri (University of

Insubria, Italy) and Mandela Toku (RWESCK, KNUST, Ghana)

Francesco Colombo (University of Modena) was the winner of the Lodovico prize for the "most active student inside and outside the lecture hall".

Feedback from participants was overwhelmingly positive. They appreciated the depth and breadth of the topics covered, the quality of lectures, and the interactive nature of the workshops. The event succeeded in fostering a dynamic and collaborative learning environment, with many participants expressing a desire for similar future events. They also provided some constructive comments to improve the lectures and workshops,

that will be considered for the next editions of the school.

Special social event

On June 5th, the participants celebrated the 50th anniversary of the Erice School. This special event started with the "Guess the crystallographer" challenge, where teams were asked to identify a well-known crystallographer by following the hints provided by the quizmaster. This was followed by dinner, a special celebratory cake as well as awards to the best golden artefact created by the students. Both social events underpinned the main value of the School: enabling personal contact between experts and students, that builds and nurtures the crystallography community.



Participants, lecturers, and organisers gathered in San Francesco for a group picture.

Report on the ETH-EPFL summer school on synchrotron diffraction and scattering for advanced materials research held at the BM01 beamline of the ESRF

By Pattaraphon Rodlamul^a, Benjamin Aymoz^{b,c*}, and Nora Zimmerli^{d*}

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^bETH Zürich, Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, 8093 Zürich

^cEMPA, Laboratory for Thin Films and Photovoltaics, 8600 Dübendorf

^dETH Zürich, Laboratory of Energy Science and Engineering, Department of Mechanical and Process Engineering, 8092 Zürich

*Correspondence: norazi@ethz.ch, baymoz@ethz.ch

Following the first successful BM01 Summer School in June 2023, 20 PhD students from various backgrounds, universities, and nationalities came together this May (13th-17th) for another week packed with scattering, diffraction, and socializing at the Swiss-Norwegian Beamlines (SNBL). This year's school was kindly funded by the [joint ETH-EPFL summer school program](#) and Dectris and was proposed by PhD students from both universities and supported by professors Christoph Müller, Christophe Copéret, Maksym Kovalenko (all ETHZ) and Raffaella Buonsanti, Kumar Agrawal, and Jeremy Luterbacher (all EPFL), as well as Dr. Paula Abdala (P.A., ETHZ), and Prof. Wendy Queen (EPFL). The latter were also largely involved in the organization of the school which was done in a collaborative effort between the PhD students and the staff of the SNBL (Dr. Dmitry Chernyshov (D.C.), Monique Faure, Dr. Chloe Fuller (C.F.), Dr. Charly McMonagle (C.M.M.) and Dr. Vadim Dyadkin (V.D.), Dr. Dragos Stoian, and Dr. Kenneth Marshall).

The school aimed at giving a broad overview of the possibilities of synchrotron-based diffraction

techniques can offer for advanced materials research with a special focus on the various methods available at BM01 including small and wide angle scattering, high-resolution diffraction, and reciprocal and direct space diffraction mapping. The theoretical and practical lessons were mostly presented by the SNBL staff, as well as guest lecturers Dr. David S. Wragg (D.S.W., Institute for Energy Technology, Oslo), Prof. Arkadiy Simonov (A.S., ETHZ), Dr. Pascal Schouwink (P.S., EPFL), and Dr. Paula Abdala. The school participants also did their part to demonstrate the broad applications of synchrotron scattering and diffraction by presenting their respective research topics, ranging from catalysis, batteries, and CO₂ sorbents, to additive manufacturing of metals, and building materials.

D.C. provided insight on how synchrotron radiation is generated, used for various experimental techniques, and the preparation of successful beam time proposals, whereas C.M.M. discussed the variety of possible experiments at the



beamline, highlighting the advanced sample environments developed by the staff. C.M.M. and V.D. guided students through the necessary software pipelines for data collection, processing, and analysis. The invited lecturers seized the opportunity to engage with the new generation of synchrotron users, illustrating through their experiences how the BM01 beamline benefits the Swiss materials science community. P.S. addressed surface and microstructure analyses, whereas A.S. demonstrated the role of diffuse X-ray scattering in understanding structural disorder. Complementarily, P.A. and D.S.W. showcased the advantages of synchrotron radiation for time-resolved experiments in *in situ* studies of catalytic processes and *operando* observations of battery cycles.

Furthermore, the beamline scientists of BM01 and BM31 provided an engaging tour of their experimental setup, linking theoretical explanations to practical experiments. During the second half of the school, students were given the

chance to perform their own data collection and analysis on samples related to their respective research projects. Each student also had the opportunity to work with various sample types, including powders, thin films, and single crystals.

Throughout the week, students were frequently mixed into different groups with beamline scientists, fostering productive discussions, especially following the brief presentations of their research projects. The week-long summer school culminated in a memorable dinner at a traditional Grenoble restaurant, bringing together participants, speakers, and SNBL staff. Undoubtedly, the scientific insights and social connections formed during the week will serve as valuable assets for the students' careers and benefit the Swiss scientific community

Last words from the authors

Organizing and participating in the BM01 school on synchrotron diffraction

and scattering was a great opportunity and learning experience that would not have been possible without the exceptional efforts of all the organizers, particularly the SNBL staff (Dmitry, Chloe, Charly, Vadim, Monique, Wouter, Dragos, and Kenny), Paula Abdala, and Wendy-Lee Queen. Our sincere thanks again to them!

SGK/SSCr Travel Grants 2024 – First Semester

We congratulate Landuyt Annelies Landuyt on her travel award and her successful participation at MRS Spring Meeting 2024.

April 22-26, 2024 MRS Spring Meeting, Seattle, Washington, USA

by Landuyt Annelies



The 2024 MRS Spring Meeting in Seattle was a vibrant and extensive event, bringing together researchers from around the globe to discuss the latest advancements in materials research. The conference covered a broad spectrum of topics, from nanomaterials and biomaterials to energy materials and advanced characterization techniques. Attending such a large and interdisciplinary conference dedicated to materials research was an enriching and inspiring experience, providing a unique opportunity to learn about cutting-edge developments and network with fellow researchers.

As part of the "Advanced Characterization of Energy Materials"

session, I presented our in situ synchrotron XRD-based work on the role of Na_2CO_3 in accelerating the CO_2 uptake kinetics of MgO-based sorbents. It was a great pleasure to present the work to an audience of researchers with expertise in different X-ray and electron-based characterization techniques, offering new perspectives and ideas for future studies. Particularly, I found the talks by Prof. Qian Chen and her students very inspiring. She and her students presented groundbreaking research ranging from 4D-STEM imaging of the evolution and performance relevance of microstructures in cathode nanoparticles to the liquid-phase TEM study of the dynamics of nanoparticles. Apart from the Advanced Characterization sessions, I also attended several sessions on crystal growth as well as sessions on dynamics using X-rays. The Crystal Growth sessions offered fascinating insights into the fundamental processes of nanocrystal growth as studied by liquid-phase TEM and small-angle X-ray scattering (SAXS). I also had the privilege of attending an interesting talk by Prof. James J. De Yoreo, a pioneer and leader in the field of the physics of crystal nucleation and growth. Furthermore, there was an intriguing presentation on how researchers solved the 200-year-old geology mystery of dolomite growth using out-of-the-box thinking and theoretical calculations.

Overall, attending the MRS Spring Meeting 2024 was an invaluable

experience. It broadened my perspective, provided me with new insights and ideas, and laid the foundation for possible future

collaborations. I am deeply grateful to the SSCr board for their support in making this trip possible.

2024 Crystallographic Howard Flack Lecture Series: cancelled

We regret to inform you that the 2024 Crystallographic Howard Flack Lecture Series has been cancelled. Unfortunately, Nobel Laureate Dan Shechtman from Technion, Tel Aviv, is unable to make the trip this year.

We appreciate your understanding and hope to bring an exciting program for the 2025 edition. Thank you for your continued support and interest in the Howard Flack Lecture Series.

Sincerely,
The SSCr Board

Minutes of General Assembly 2023

Swiss Society for Crystallography SGK/SSCr

Friday, 08.09.2023, 13:15 – 14:15

Department of Chemistry, Irchel Campus, University of Zürich, Winterthurerstrasse 190, 8057 Zürich

Agenda:

1. Quorum (Art 12, by-laws, count members only)
2. Minutes of GA 2022 (Bern), proposal for acceptance (p. 37-45, N110)
3. Reports
 - a) Annual report
 - b) Delegates to adhering bodies (IUCr, ECA, IOCG)
 - c) Annual financial statement (2022)
 - d) Budget for next year (2024)
4. Elections
 - a) Chairperson for elections
 - b) Confirmation of current board members
 - c) Nomination of new board members: Nicola Casati (PSI) (To be submitted to the president 10 days prior to GA)
 - d) Election/confirmation of auditors
 - e) Confirmation of delegates to SCNAT, ECA, IUCr, SSC and IOCG
5. Annual Meeting and General Assembly 2024

Minutes:

- 1- Quorum and formalities

The General Assembly was chaired by Pascal Schouwink, President, 13:30 h – 14:25 h

The agenda was sent by e-mail (swiss.crystallography@gmail.com) on the 16.08.2023.

The secretary Paula Abdala, ETH, was appointed as keeper of the minutes.

With 31 members being present at this assembly, the necessary quorum of 10% (18) is reached to constitute a quorum (Art. 12).

As of 08.09.2023, we have 191 records in our database of 05.09.2023

They are grouped as:

- 14 Libraries
- 11 Corporate members (2 entries in 2022)
- 166 personal members (F + S + H)

New entries: 2022: 10; 2023: 18

Members that have not paid the annual fees for more than 3 years and could not be contacted have been removed from database.

- 2- **Proposition for acceptance of “Minutes of the General Assembly 2022, University of Bern”**

The General Assembly was chaired by Pascal Schouwink, President, 13:30 h – 14:25 h.

The agenda has been published in the Newsletter 110 on 14. August 2022 (Art. 11).

The secretary Antonio Cervellino, PSI, was appointed as keeper of the minutes.

The minutes are reported in the Newsletter issue No. 110, August 2023.

Voting: were approved unanimously, without abstention.

3- Activity report

The President, Pascal Schouwink, provided an overview of the key activities of the board of the SGK-SSCr in the past year.

Travel grants and prizes

Travel support has been awarded to five young members for conferences, workshops, and schools in 2023, and the President encourages becoming an SSCr member and to apply for travel grants. Note that PhDs and Postdocs under 35 years old are eligible to apply. The SSCr PhD prize is announced during this meeting.

Howard Flack Crystallographic Series

The Howard Flack Crystallographic Series' 4th edition in 2022 was a success featuring the lecture on Electron Crystallography by Dr. Lukáš Palatinus from FZU, Czech Academy of Sciences. There is also an advertisement for the upcoming 5th edition in 2023 which will cover Local Order and Pair Distribution Function Analysis - Total Scattering and AI approaches, by Simon Billinge. Proposals for topics for the 2024 series can be submitted at swiss.crystallography@gmail.com.

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New Activity: The SSCr Topical Workshop

As a satellite of this meeting, a SSCr Topical Workshop on Small Angle X-ray Scattering was held, and there are plans to make this an annual event, with PDF analysis in 2024. The workshop received 63 registrations, and the SCNAT support was 2.5 kCHF. Speakers at the event were Antonia Neels (EMPA), Stefan Salentinig (Uni Fribourg), Vivian Lütz Bueno (PSI), Thomas Weber (ETHZ), Heiner Santner (Anton-Paar), Carlotta Giacobbe (Xenocs), and Brian Pauw (BAM).

Report on the 26th Congress and GA of the IUCr, Melbourne from August 22-29

The 26th Congress and General Assembly of the IUCr, held in Melbourne from August 22 to 29, was attended by approximately 1800 participants. There were 3 plenary lectures and 29 keynote lectures, including 2 from Switzerland: Oksana Zaharko from PSI and Simon Grabowsky from Bern. Prizes were awarded to Wayne Hendrickson for the Ewald Prize and Jian-Min Zuo for the Gjønnes Medal. The 2023 Bragg Prize was awarded to Arkadiy Simonov

Other key points highlighted in the report include the admission of the African Crystallographic Association (AfCA) into the Union, a motion to suspend the Membership of the Russian Academy of Sciences as Adhering Body of the IUCr being declined, a financial crisis of the IUCr leading to an investigation to move the Union's domicile from Geneva to the U.K. and from USD to GBP, and the election of Santiago Garcia-Granda from Spain as the new President.

There were also changes in the commissions, with new appointments and ad interim positions for Materials, Magnetic Structures, Powder, and Quantum Cryst. Commissions. Future conferences were announced for the years 2026, 2029, and 2032 in Calgary, Berlin, and Xi'an, China, or Jeju, South Korea, respectively.

Additionally, a satellite workshop titled "A practical approach to synchrotron experiments" was successfully organized by Dubravka Sisak-Jung for the SSCr. This workshop provided a platform for beamline scientists from various fields and users to

exchange valuable insights, and there was positive feedback encouraging the continuation of such sessions in the future.

The SNBL Summer School was mentioned, that was held between 05-09 June 2023, with 16 participants. The chair was Dr. Dmitry Chernyshov, and lectures were given by BM01 staff. Coordination and financial support: Prof. Wendy Lee Queen (EPFL) and Dr. Paula Abdala (ETHZ/SSCr) – Swiss delegates at the SNBL council.

3c) Annual financial report

Enrico Giannini (Treasurer) presents the closing of the financial year 2021 and the financial situation in 2022.

Summary SGK Finances 2022

	CHF
Total 31.12.2021	55'189.67
UBS account	45'654.72
Cash on hand	515.55
Total 31.12.2022	46'170.27
Balance	-9'019.40

Report of revisors:

The financial report 2022 has been approved by the auditors B. Spingler and A. Neels

Revisorenbericht für die Jahresrechnung 2022 der Schweizerischen Gesellschaft für Kristallographie (SGK)

Konten:

UBS UBS 279-C0291110.0

Die Unterzeichneten haben Kenntnis genommen von der Jahresrechnung der Schweizerischen Gesellschaft für Kristallographie. Die Rechnungsprüfung betrifft die Periode vom 1. Jan. 2022 bis 31. Dez. 2022. Die Unterzeichneten stellen fest, dass die Abrechnung mit den vorgelegten Belegen übereinstimmt.

Am 31. Dez. 2022 ist der Stand der Konten und der Kasse:

UBS	SFr.	45'654.72
Kasse	SFr.	515.55
Summe SGK	SFr.	46'170.27

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

Ort / Datum
Genève, 15.02.2023

Unterschriften



B. Spingler
(Universität Zürich)



A. Neels
(EMPA Dübendorf)

SGK Financial Report 2022

Income:

Membership dues:

Full members (various amounts due to debts)

56x40 + 1x50 + 11x80 + 2x120 + 1x198.31

3'608.31

Students 11x10 + 1x20

130.00

Companies 6x130

780.00

Total membership

4'518.31

Subsidy SCNaT (2021)

7'000.00

Total Income 11'518.31

SGK Financial Report 2022

Expenses:

Annual Meeting

3'000.00

Zurich School of Crystallography

2'000.00

Howard Flack Lecture Series

1'801.75

SSCr scholarship for Ukrainian student

7'500.00

Travel Grants (including PhD prize)

2'000.00

Travel costs of ECA/IUCr/IOCG delegates

1'500.00

Membership dues to SCNat (160 members at 01.01.2022)

1'120.00

Association to ECA

183.56

Printing and publishing costs (newsletter)

1302.00

Bank expenses

130.40

Total Expenses

20'537.71

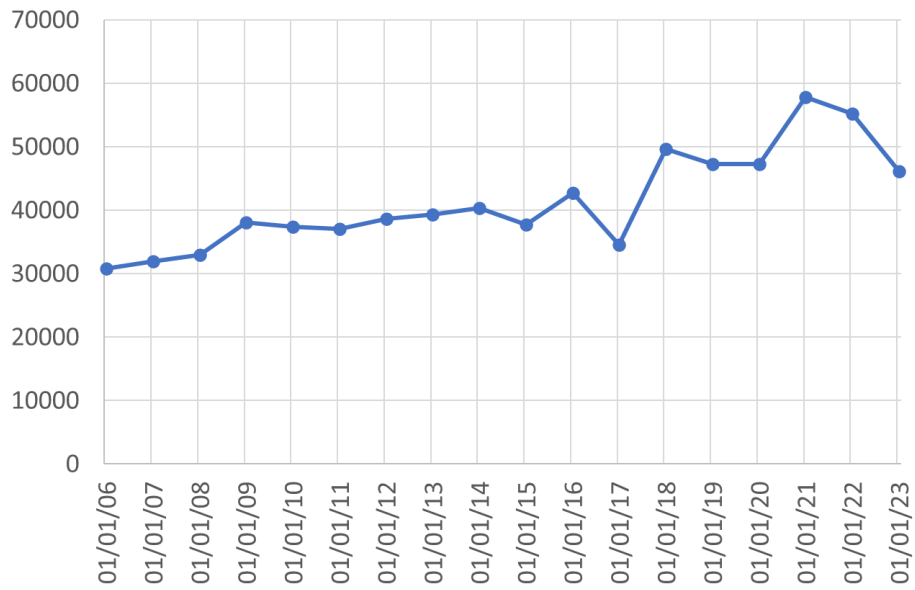
Expenses

**Income –
- 9'019.40**

Fluctuation of the membership dues



Capital of the SGK (CHF)



SGK financial situation 2023

Credits:		Debits:	
Membership dues (until 31/08)	6'752.88	PSI School (to be paid)	2'000.00
SCNat contribution 2022	9'801.75	SGK annual meeting (+ poster prize)	3'000.00
Sponsorship for event organization	1'500.00	SAXS workshop	300.00
		IUCr satellite workshop (catering)	232.05
		IUCr satellite workshop (speakers)	1'500.00
Total Income	18'054.63	Flack Lecture series (expected)	4'000.00
		Travel grants for students	1'500.00
		IUCr and ECA delegates	1'000.00
		IOCG delegate	500.00
		Membership dues to SCNat	1'057.00
		Bank charges	71.47
		Publication costs	705.05
		ECA membership	176.05
		Total Expenses	16'041.62

3d) Budget for 2024

SGK Budget proposal 2024

Credits:		Debits:	
Membership dues	5'000.00	SGK Annual meeting + poster prize	3'000.00
SCNat - contribution for SGK annual meeting		SGK support to Zurich School	2'000.00
	2'500.00	Travel Grants for Young Scientists	3'000.00
SCNat – Zurich school of crystallography	2'000.00	Howard Flack Lecture Series	4'000.00
SCNat - PhD / master students travel grants	2'000.00	International School in Erice	1'500.00
SCNat - Crystallographic Lectures:		SSCr students workshop on PDF	2'000.00
Howard Flack Lecture Series	2'000.00	Sponsoring and event advertisement	
International School in Erice	1'000.00	(posters, flyers, webpage)	500.00
SCNat - SSCr students workshop on PDF	2'000.00	Membership dues to SCNat	1'100.00
SCNat - Publication costs	500.00	ECA national membership dues 2023	200.00
		Publication costs	1'200.00
Total Income	17'000.00	Bank charges	200.00
		Total Expenses	18'700.00
		Income – Expenses	-1'700.00

Membership fees 2023:

Regular membership fee: CHF 40 / year

Student membership fee: CHF 10 / year

Corporate membership fee: CHF 130 / year.

It is proposed to maintain the same membership fees for the year 2023.

As per the bylaws, the Assembly is required to vote on the presented financial reports and membership fees.

VOTING: The Annual financial report 2023, presented by the Treasurer Enrico Giannini, is approved unanimously, without abstentions.

VOTING: The Budget forecast 2024, presented by the Treasurer Enrico Giannini, is approved unanimously, without abstentions.

VOTING: The prolongation of the current fees for 2024 is approved unanimously, without abstention.

Elections

- a) Definition of a chairperson for the elections

The chair for the elections is the Vice President, Simon Grabowsky.

Confirmation of current board members

- **P. Abdala, E. Giannini, S. Grabowsky, P. Schouwink, D. Sisak-Jung**

VOTING: The present board members are confirmed unanimously, without abstentions.

- b) New nominations to the board:

Nicola Casati (PSI)

VOTING: Nicola Casati is accepted as a Board member unanimously, without abstentions.

- b) Confirmation of auditors:

Antonia Neels, Bernhard Spingler

VOTING: Bernhard Spingler as Auditor confirmed, and Antonia Neels as Auditor is replacing Kurt Schenk.

- c) Confirmation of delegates to ScNat, ECA, IUCr and IOCG

- ScNat: P. Schouwink (automatically assigned to acting president)
- ECA: A. Linden (Zurich, until 2024 then automatically assigned to vice-president)
- IOCG: E. Giannini (Geneva)
- IUCr: S. Grabowsky (Bern), P. Schouwink (Lausanne)
- SSC-SNBL: S. Grabowsky, P. Schouwink
- Delegates to ECA, IUCr and IOCG are financially supported by ScNat (500 CHF/delegate) to attend their general assemblies. The eligible GA are considered to take place at ECM, IUCr-congress and ICCGE

VOTING: The proposed delegates are approved unanimously, without abstentions.

- 4- **2024 Meeting and General Assembly. Decision on location and date: Basel September 13th (Dinner Sep 12th)**




5- Other motions of members and communication




- f) Newsletter: can we stop printing?
No unanimous decision was made.




Minutes written by the Secretary, Paula Abdala, and approved by the President, Pascal Schouwink.




Calendar of Events




 **ECM34: 34th European Crystallographic Meeting**
26-30 August 2024
 Padova, Italy
 WWW.ECM34.ORG

 **EPDIC18: The 18th European Powder Diffraction Conference**
August 30th to September 2nd, 2024
 Padova, Italy
 <https://epdic18.org/>

Workshop on Tips and tricks for the crystal growth of inorganic materials
 26-27 of August 2024
 Villigen, Switzerland
 <https://indico.psi.ch/event/15694/>

 **Summer School "Kristallographie" 2024**
16- 20 Sep 2024
 Warendorf, Germany
 <https://www.tu-braunschweig.de/iaac/zentrale-einrichtungen/roentgenstrukturanalyse/sommerschule-kristallographie>

 **INTERNATIONAL SCHOOL of CRYSTALLOGRAPHY: Electron Crystallography**
30 May - 7 June 2025
 Erice, Italy
 <https://crystalerice.org/2025/>

 **INTERNATIONAL SCHOOL of CRYSTALLOGRAPHY: Quantum Crystallography**
30 May - 7 June 2025
 Erice , Italy
 <https://crystalerice.org/2025/>

In-situ structural biology: expanding the toolbox for structural cell biology



4-7 February 2025



Heidelberg, Germany



<https://www.tu-braunschweig.de/iaac/zentrale-einrichtungen/roentgenstrukturanalyse/sommerschule-kristallographie>

ESRF User Meeting 2025



10 - 12 February 2025



Grenoble, France



<https://www.esrf.fr/home/events/conferences/2025/user-meeting-2025.html>

Sagamore XX Conference on Quantum Crystallography



10 -15 November



Delhi NCR, India



<https://www.snu.edu.in/conferences/Sagamore2024>

Calls for proposals at large scale facilities

Beside normal proposals, most facilities allow urgent beam time requests. Please check directly with the facility. (tba = to be announced)

Facility	Deadline(s)	Link
SLS		
All except non PX	suspended	
Protein crystallography (PX)	suspended	
SINQ/SLS	suspended	
Joint x+n proposals (MS/HRPT)		
SINQ		https://www.psi.ch/de/useroffice/proposal-deadlines
All instruments regular calls	15.05, 15.11	
SμS: Swiss Muon Source		
DOLLY, GPD, GPS, HAL-9500, LEM	01.06, 01.09	
SwissFEL		
ARAMIS-Alvra, ARAMIS-Bernina	15.03, 15.09	
ESRF		
Standard proposals	01.03, 10.09	http://www.esrf.fr/UsersAndScience/
Long Term Project and HUB proposals	16.01	
CRG SNBL	01.03, 10.09	www.esrf.fr/UsersAndScience/Experiments/CRG/BM01# For more details on the access mode to SNBL: wouter@esrf.fr
ILL	tba	www.ill.eu/users
FRM II	tba	http://www.mlz-garching.de/user-office/
All instruments/ Rapid access program		
SNS Oak Ridge	30.08	http://www.neutrons.ornl.gov/users/proposal-calls
DESY	tba (typically 01.03 01.09)	https://photon-science.desy.de/users_area/calls_deadlines/index_eng.html

Information about Travel Grants for SSCr Members

Our Society is supporting members participating at international conferences, workshops and schools.

Conditions for travel grants for young SSCr members (under 35):



- Only current members of the SSCr can be supported financially (annual membership must be paid).
- Student members can get up to CHF 500 for a poster presentation and CHF 750 for an oral presentation. Attendance at a workshop or school outside Switzerland, if the program does not permit participant presentations, can be supported with CHF 500.
- Postdocs can be supported only for oral presentations with a maximum of CHF 500.

Per institute and year, a maximum of two persons can be supported.

How to apply?

Please submit applications to the SSCr board via swiss.crystallography@gmail.com including the following:

- conference abstract if applicable, type of presentation/involvement and letter of motivation
- letter of support from your supervisor
- brief budget of expected costs of attending the meeting
- specify the date you first joined the SSCr

A 1-2 page scientific report for the SSCr newsletter is expected within 2 months after the meeting which will be published in this newsletters.

Travel grants for retired SSCr members

Financial support can also be granted to retired SSCr members under the following conditions:

- Active participation at an event is required: e.g. presentation, lecture, session chair, organizer
- Young researchers have priority if our budget is limited
- The grant amount will be decided by the board, depending on the available budget

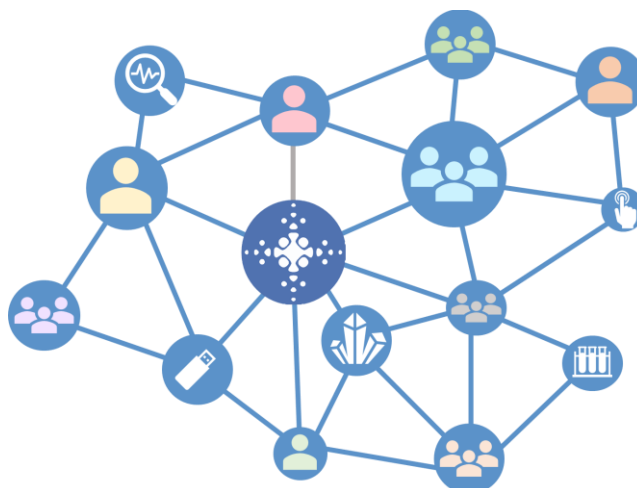
Institutional members and supporting institutions

Corporate members



Supporting institutions

Become a member of the SSCr!



- ✓ Connect with researchers, scientists, and students from across scientific fields.
- ✓ Take part in events organized by the society.
- ✓ Drive the future activities of the society.
- ✓ Benefit from travel grants and PhD awards.
- ✓ Benefit from a network providing access to new collaborations and infrastructure.
- ✓ Stay up to date on upcoming events.

For more information as well as online registration, please go to our website <https://swiss-crystallography.ch/en/membership>

The yearly membership fee is CHF 40 for regular members and CHF 10 for students. SGK/SSCr is a member of the Swiss Academy of Science.

Connect with us!

Web: swiss-crystallography.ch

E-mail: swiss.crystallography@gmail.com

 [Swisscrystallog](#)

Members of the Board of the SSCr for the period 2023 – 2024



Pascal Schouwink
President
EPFL Valais Wallis



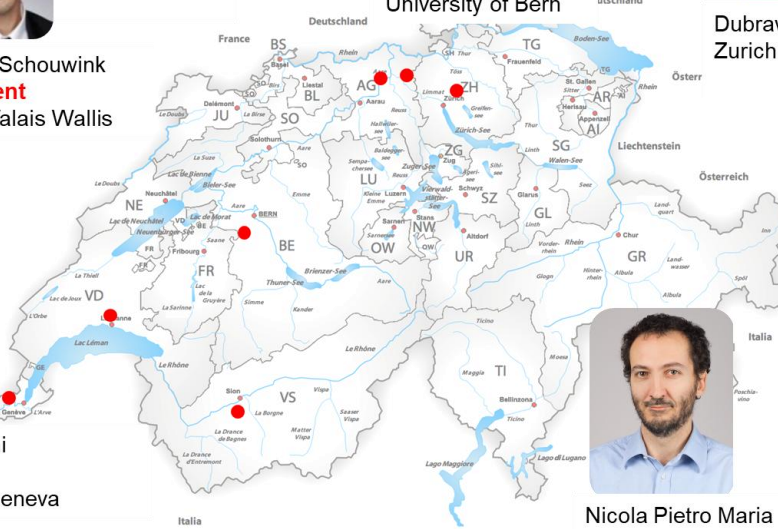
Simon Grabowsky
Vice-President
University of Bern



Dubravka Sisak
Zurich Instruments



Enrico Giannini
Treasurer
University of Geneva



Paula Abdala
Secretary
LESE-ETHZ



Nicola Pietro Maria Casati
Events organization
Material Science Group PSI

Candidate for the next period:



Céline Besnard
University of Geneva

Auditors:



Prof. Dr. Bernhard Spingler
University of Zurich



Prof. Dr. Antonia Neels (EMPA)

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SGK/SSCr Newsletter (ISSN 1662-5358, online version: ISSN 1662-534X)

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BLZ: 279

Printing and

Mailing:



Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

The newsletter of SGK/SSCr is published 2-3 times a year with a circulation of 250. Contributions are welcome at any time, as well as illustrations for the cover. Articles in English, German or French may be submitted. Please send all interesting material directly to the editor.

Commercial advertisements of material of interest to members of the SGK/SSCr are welcome. Please contact the treasurer for details of the advertising rates.