

dispersion experiment to show the relationship between some basic experimental variables and their influence on phasing and on an uninterpretable map or a map where the main chains can be auto-traced. Overall these results suggest a more optimal sulfur SAD experiment ie based on a complete description of the crystal system and the instrument to be used for data collection.

Keywords: SAD, wavelength, radiation damage

MS.11.1

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Hands-on crystallographic teaching: The Zurich School of Crystallography - Bring your own crystals

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The Zurich School of Crystallography, initiated by the authors in 2007, teaches the theory of small-molecule crystallography, and offers full hands-on experience from data collection to structure refinement and analysis of results. Our speciality is to give students the opportunity to bring crystals of a compound of interest in their current research and to return home with their completed structure. This ambitious concept relies on several key conditions:

Know what you want to achieve: Our aim is to introduce non-specialists to routine single crystal structure determination, rather than to create the next generation of expert crystallographers. The students learn to conduct routine structure analyses competently and to recognise when to ask for expert advice.

Know what you want to teach: We focus on small-molecule crystallography and inform applicants of the course content in order to avoid false expectations. Participation of students specifically interested in macromolecular or powder methods is discouraged.

Ensure students understand the objectives of the school: We make it clear beforehand that we do not run a data collection service nor solve problem structures. We ask for the students' crystals in advance, screen them for suitable quality and didactical usefulness and collect preliminary data.

Maximize the motivation of the students: Working on their own crystals ensures strong interest by the students. Access to a diffractometer of the student's choice and individual computing facilities are important. A student:tutor ratio of 2:1 ensures no-one gets left behind. Consequently, we limit the school to 20 students.

Have the equipment available: 5 diffractometers (4 different types) are used. There is one personal computer per student with all of the required software.

Keywords: crystallographic teaching, teaching of crystallography, structure determination

MS.11.2

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Conquering superspace - A beginner's guide to modulated structures

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In the daily routine of a crystallographer modulated structures are often still perceived as an unpleasant disturbance. Their diffraction pattern, characterized by the existence of additional (satellite) reflections, requires (3+d) indices for an integer indexing, a complication usually resulting in an immediate dismissal of the crystal under study. Another obstacle may be the unfamiliarity with the so-called superspace approach, a concept developed to overcome the above mentioned loss of 3-dimensional periodicity and allow for a correct description of modulated structures. The theoretical foundation for the superspace approach is well-established by now. Also considerable efforts have been put into making the software package JANA2006 which can conveniently handle data and structures of modulated compounds available and user-friendly [1]. What still seems to be missing somehow are illustrative examples of molecular compounds which can be used to demonstrate in a comprehensible way how to approach modulated structures. In this context we will present a selection of cases from our pharmaceutical service lab along with a detailed recipe how to handle the modulated structure of a typical organic compound [2]. Having established a working knowledge of the concept and terminology of the superspace approach we will discuss various aspects of indexing, data processing and scaling as well as structure solution, refinement and interpretation details. Finally, the validity of a (classical 3-dimensional) superstructure approach and additional quality control features in JANA2006 are described.

[1] V. Petricek, M. Dusek, L. Palatinus, JANA2006, Institute of Physics, Praha, Czech Republic (2006).

[2] T. Wagner, A. Schoenleber, K. Baumann, *Acta Crystallogr.* A63, s51 (2007).

Keywords: modulated structure, superspace, teaching

MS.11.3

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Sustaining crystallography in the 21st century: Education policies and use of cyberinfrastructure

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The USNC/Cr conducted two surveys to determine the status of crystallography education and training in the US, in both physical and life sciences. The ACA and USNC/Cr then held an education summit, the outcome of which is a consensus policy statement on crystallography education and training that makes recommendations for a comprehensive re-evaluation of crystallography education, provides guidelines to professional societies and academic departments for crafting future crystallography curricula, and suggests ways to develop in the broader scientific community an appreciation for the value of crystallographic information. With the migration of academic crystallography from a research specialty to a technique employed by a wide community of users, instruction in crystallography is increasingly relegated to non-curricular resources, such as web-based tutorials. While such tutorials often are well-constructed and provide a valuable resource to the broader scientific community, they generally do not provide practical experience needed to appreciate the value of crystallographic information and correctly interpret and judge the quality of crystallographic results. We can now exploit advances in cyberinfrastructure to effectively broaden access to instrumentation, data handling and analysis. These advances can develop in the wider user community a sufficient working knowledge of the field, enabling them to answer specific

research questions, collaborate with those having greater expertise, utilize crystallographic results as the basis for or validation of their own work, and critically review published structures or those being submitted for publication. Opportunities, challenges and pedagogical implications presented by these policies and cyber instruction will be discussed.

Keywords: teaching, policy, cyberinfrastructure

MS.11.4

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Use of images from neolithic art, clip art, digital cameras, and MATLAB® in teaching crystallography

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Images illustrating symmetry are valuable in the teaching of crystallography. Unusual two-dimensional wall-paper patterns from Neolithic art collected by Prof. Slavik Jablan will be shown. Amazing illustrations of two-dimensional point groups and space groups have been constructed by students using clip art with programs such as Microsoft Paint. Digital cameras can be used to collect imaginative examples of crystallographic interest such as reflections in ponds, spiral-staircase screws, and footprints-in-the-sand glide planes. Advanced computer languages like MATLAB® can be used to create parametric figures such as spirals, seashells, and butterflies (T.H. Fay *Amer. Mat. Mon.* 96, 443, 1989) which then can be inserted in space groups. Illustrations will show teaching examples and student exercises, many from *Foundations of Crystallography with Computer Application* by Maureen M. Julian, CRC press 2008.

Keywords: crystallographic education, computer-aided instruction, symmetry

MS.11.5

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Teaching crystallography: Approaches for non-crystallographers and non-native speakers in Asia

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The teaching of crystallography, as a cross-disciplinary science, is required in a variety of subject areas and at different academic levels. Some of the approaches and curricula of crystallography developed at a technological university in Asia, and given at the undergraduate or introductory level in Solid State Chemistry and Materials Science and Engineering, as well as at the post-graduate level in a one-semester course on Chemical X-ray Crystallography are reviewed. The needs of non-crystallographers, and even non-native speakers, can pose additional challenges for successful teaching and learning outcomes. The use of visual constructs and in-class exercises to develop understanding is thus emphasized. The fundamentals of crystallographic symmetry and both powder and single crystal diffraction can be tackled via case studies of increasing complexity, starting from 2D patterns and progressing through simple 3D inorganic structures to complex organic or protein molecular packing arrangements. At more advanced level the conceptual background seems best augmented by combination with experimental practice.

The Asian region has some of the most disparate levels of educational and scientific resources in the world. Many sizeable countries within it do not have even one single crystal X-ray diffractometer. A case is presented for the need of a workshop-based crystallographic school, with hands-on access to modern instrumentation, to promote and sustain crystallography in the less developed parts of the region.

Keywords: crystallographic teaching, inorganic and organic crystal structures, materials engineering teaching programme

MS.12.1

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X-ray scattering studies of liquid-crystalline suspensions of anisotropic mineral nanoparticles

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Mineral liquid crystals are colloidal suspensions of anisotropic (disc-like or rod-like) mineral nanoparticles in a solvent, usually water. These suspensions form various types of liquid-crystalline nematic, lamellar, or columnar phases, depending on the particle anisotropy and concentration. Such phases combine long-range orientational order of the particles with either short-range positional order or long-range positional order in 1 or 2 dimensions. X-ray scattering is a very well suited technique to study these properties because it gives direct access to the nematic order parameter, and to the dimensionality and symmetry of the positional order. This will be illustrated by various examples: Suspensions of goethite (FeOOH) nanorods provide a very convenient system because it displays all the above-mentioned phases [1,2], sometimes coexisting in a single sample [3]. Besides, suspensions of natural clays will be used to describe the case of disc-like particles [4,5]. Moreover, if time allows, I will also show how the dynamic properties of nematic suspensions of rod-like nanoparticles can be probed by the rather new technique of X-ray photon correlation spectroscopy (XPCS).

[1] B.J.Lemaire et al, *Phys. Rev. Lett.*, 88, 125507 (2002).

[2] B.J.Lemaire et al, *Phys. Rev. Lett.*, 93, 267801 (2004).

[3] G.J.Vroege et al, *Advanced Materials*, 18, 2565 (2006).

[4] L.J.Michot et al, *Proc. Nat. Acad. Sci. USA*, 103, 16101 (2006).

[5] L.J.Michot et al, *Langmuir*, 24, 3127 (2008).

Keywords: liquid crystals, colloids, small-angle scattering

MS.12.2

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Crystallography of 2D and 3D structures in liquid crystal amphiphiles and nanocomposites

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A combination of X-ray diffraction methods was used to study thermotropic phases of three groups of liquid crystalline materials. The different experimental and analysis techniques used will be illustrated on selected examples. Firstly, a wide range of T-shaped, X-shaped and π -shaped amphiphiles with three or four incompatible moieties were studied. A range of novel phases with 2D and 3D