

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

Anthony Linden<sup>1</sup>, Hans-Beat Buergi<sup>2</sup>

<sup>1</sup>University of Zurich, Institute of Organic Chemistry, Winterthurerstrasse 190, Zurich, ZH, CH-8057, Switzerland, <sup>2</sup>Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland, E-mail: alinden@oci.uzh.ch

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

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#### Conquering superspace - A beginner's guide to modulated structures

Trixie Wagner<sup>1</sup>, Andreas Schoenleber<sup>2</sup>

<sup>1</sup>Novartis Pharma AG, Novartis Institutes for BioMedical Research, WSJ-503.12.08, Basel, Basel, 4002, Switzerland, <sup>2</sup>Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany, E-mail: trixie.wagner@novartis.com

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

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

Katherine A Kantardjieff<sup>1,2,3</sup>

<sup>1</sup>California State University Fullerton, Chemistry and Biochemistry, 800 N. State College Blvd., Fullerton, CA, 92834-6866, USA, <sup>2</sup>W.M. Keck Foundation Center for Molecular Structure, <sup>3</sup>United States National Committee for Crystallography, E-mail: kkantardjieff@fullerton.edu

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