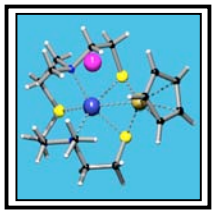
The Zürich School of Crystallography

Bring Your Own Crystals



University of Zürich

June 9 - 22, 2013

The fifth Zürich School of Crystallography took place, as usual, within the Institute of Organic Chemistry at the University of Zürich (UZH). The 19 enthusiastic participants from diverse corners of the world were inducted into the essential theory and practical aspects of small-molecule single-crystal X-ray crystallography. All aspects of the School ran very well with no hiccups and the enthusiasm of the participants remained high throughout, even though they find the School very intense. We maintained our usual 2:1 student:tutor ratio and participants always comment very favourably on the personalised friendly attention they receive. The participants this year comprised 1 MSc and 13 PhD students, 1 postdoc, 1 young academic, 2 more senior academics and 1 researcher. They came from 15 countries: Canada, Finland, Ghana, Italy, India, Nigeria, Poland, Romania, Slovenia, Switzerland, Sweden, Thailand, Turkey, The Ukraine and Uzbekistan; 8 women and 11 men, with ages ranging from 24 to 50. It is pleasing to see increasing interest from some African, Eastern European and Central Asian countries. The 10 tutors were from the Universities of Basel, Bern, Geneva, Zürich, the EPFL Lausanne, the ETH Zürich and the Institute of Physics, Prague.

The participants worked very hard throughout the School. The daily schedule of alternating lecture blocks and practical work in both the morning and afternoon sessions allows the participants to assimilate the theory and practical aspects readily. The practical work included hands-on experience in groups of two at one of the five diffractometers available in the various chemistry institutes at the UZH and ETH Zürich. The tutorial exercises and structure refinements were done in the computer classroom of the Institute of Organic Chemistry,

UZH. We give the participants two real-case example data sets to cut their teeth on; they learn to use the software and to recognise and resolve unexpected difficulties with structures. Each participant then solved the structure of the compound they had provided crystals of in the lead-up to the School. In this way, they get excited about being able to solve the structure of a compound of specific interest to them. The supplied samples again provided a wide range of sample types (organic, organometallic, coordination polymer, natural product and mineral) and some interesting and demanding challenges, such as twinning, disorder, disordered solvent molecules, and unusual or ambiguous space groups. All participants were able to complete their structures successfully.

On the final day of the School, each participant gave a ten minute presentation on their own structure. Those desiring credit points had to sit a two-hour written exam while the remainder also took the exam to self-test their knowledge. Each day concluded with short discussion where participants can express their feelings about their experience that day. We also offer a repetition lecture slot where the topics can be nominated by participants who feel that they did not quite grasp a certain aspect the first time. Relaxation times and breaks benefited from the pleasant environment of the university campus and surrounds. Interesting discussions with the tutors often continued over the evening meal. Social events included a mixer, barbeque and a half-day excursion to the Swiss Light Source and SINQ neutron spallation facility of the Paul Scherrer Institute.

The central goal of the School is to equip each participant with enough knowledge of the theory and practice of X-ray diffraction and single-crystal small-molecule structure determination so that they could competently determine their own structures when they return to their home laboratory. With this in mind, the practical sessions and example structures are designed to allow the participants to see behind the button-pushing and learn about the actual procedures going on when various operations are performed, and then how to interpret whether or not the appropriate result has been obtained and other signs of success or unresolved problems.

At the end of the School, every participant completed a questionnaire. Very positive feedback was received about the quality of the School overall, the friendliness, accessibility and approachability of the tutors, the organisation, the venue and the accommodation. Participants often suggest including more example structures in the practical work, but course time is limited and already intense and we believe a balance of theory and practical work is important if the participants are to receive a proper understanding of the field. During the final banquet, each participant received a certificate and a copy of "Crystal Structure Refinement, A Crystallographer's Guide to SHELXL" by Peter Müller, kindly donated by the IUCr and OUP. After two weeks together, many new friendships had been established and people did not want to part company at the end of the last evening. The personal impressions of one of the

participants are given further below. We are already planning for the next School, which will be held in June, 2015.

We are very grateful for the generosity of the sponsors: Institute of Organic Chemistry of the University of Zürich, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, International Union of Crystallography, Verlag Helvetica Chimica Acta, Oxford University Press, Agilent Technologies, Bruker AXS, Oxford Cryosystems and the X-ray Diffraction Services, CSEM, University of Neuchâtel, plus the support from the Chemistry Platform of the Swiss Academy of Sciences.

Tony Linden, Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2013 – Report from a participant

The 2013 Zürich School of Crystallography (ZSC) ran this June for 2 weeks (9-22 June) on the campus of the University of Zürich. This intense course is designed for senior graduate students or, in fact, anyone interested in learning the background and techniques of modern crystallographic characterisation of small molecules or intermetallics. This years' edition featured a very strong list of lecturers / tutors assembled by Tony Linden (Editor: *Acta Crystallographica C*; U. Zürich) and Hans-Beat Bürgi (Emeritus U. Bern / U. Zürich) which included H. Flack (Emeritus U. Geneva), J. Hauser, P. Macchi (both of U. Bern), G. Chapuis (Emeritus EPFL: Lausanne), O. Blacque (U. Zürich), M. Neuberger (U. Basel), L. Palatinus (Inst. Physics, Prague) and M. Wörle (ETH: Zürich). This potent collection of experts each lectured and tutored the participants who hailed from locations across Europe, Asia, Africa and North America. This course is designed for anyone wanting to expand their general knowledge of crystallography, experience first-hand diffractometer set-up and crystal mounting, to learn the various approaches to solving and publishing small molecule crystal structures and, perhaps most importantly, to be introduced to the various pitfalls and common errors which occur in crystal structure solutions. I've been involved with X-ray diffraction before, but had never solved a structure of my own, nor did I understand the meaning of much of the data commonly reported with X-ray diffraction data. The ZSC answered all of my queries and more. The course begins with an in-depth series of lectures on the background and applications of diffraction but quickly becomes a hands-on approach to crystallography. Perhaps the best thing was the opportunity to solve my own structure after learning the basics on provided, but real, datasets. However, it is not all lectures and computer work! We spent one afternoon visiting the Paul Scherrer Institute (www.psi.ch), home of Switzerland's Synchrotron facility. We were able to see and tour the complex instrumentation and meet a number of the scientists there who are involved in X-ray, neutron and related diffraction experiments. There was also plenty of time to socialize amongst the 19 participants and their 10 tutors with frequent coffee breaks, a barbeque, wind-down time over dinner and drinks and a concluding banquet. It was wonderful to meet and get to know all the other students from very wide backgrounds and from almost every corner of the world. I'm now back at home, but very keen to solve my next dataset. The ZSC certainly provided me with all the tools I need to solve crystal structures but it has also taught me what the common mistakes are and how to recognize them. The tutors and lecturers gave a thorough and informative overview of crystallography and gave me the tools I need to solve day-to-day datasets with confidence. As a participant myself, I would highly recommend this course for anyone wanting to expand their knowledge of the subject or as a refresher course for those who might want more cutting-edge instruction in modern crystallography.

Robert Gossage, Ryerson University, Toronto, Canada