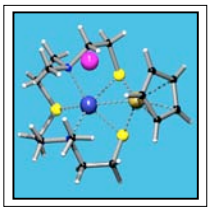
The Zürich School of Crystallography

Bring Your Own Crystals



University of Zürich

June 11 - 22, 2017

The 7th Zürich School of Crystallography was held, as usual, within the Department of Chemistry at the University of Zürich (UZH). The 20 participants comprised 1 BSc, 1 MSc and 11 PhD students, 2 postdocs, 2 junior and 3 senior academics. They came from 16 countries: Benin, China, Croatia, Finland, Germany, India, Italy, Kazakhstan, Lithuania, Mexico, Russia, Saudi Arabia, Senegal, Switzerland, Thailand, and the United Kingdom. As usual, we had our usual popular 2:1 student:tutor ratio.

All of the participants were very enthusiastic and maintained their eagerness and dedication throughout the School. Everyone mixed well and chatted eagerly together and with the tutors over the meals and during the breaks. Some were just getting their feet wet in the field of crystallography, while others were more experienced, but all came away having learned something new and feeling better equipped to tackle structure determination on their own.

We were very impressed by two young scientists from Africa (Benin & Senegal), who were not only talented and keen to learn, but also eager to take their knowledge home in order to spread the word about crystallography in their region. These participants came highly recommended by Claude Lecomte and significant bursary support, donated by the IUCr, CCDC, and UNESCO was provided in order to facilitate their attendance.

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 can 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, to learn about the actual procedures going on when various operations are performed, and to interpret whether or not the results obtained are appropriate. We successfully used the Olex^2 software once again this year and found it to be quite suitable in the School environment. The ever expanding range of

special tools and option in the program for easily handling special modelling issues, such as disorder, are very useful. The daily schedule alternated lecture blocks and practical work so that the participants could readily associate the theory with the practical aspects. The practical work included access to five diffractometers at the UZH and ETH Zürich campuses and a fully equipped computer classroom. The diffractometers included the modern Bruker Photon 100 and the newest Rigaku Oxford Diffraction Synergy instruments which are impressive in terms of speed, the availability of two radiation wavelengths and detector sensitivity.

We increased the number of real-case example data sets from two to three and some of the special features within Olex^2 were demonstrated with three additional data sets. The participants then worked on a data set collected from one of the samples they had provided. The ease of use of Olex^2 allows us to demonstrate more aspects of structure solution and refinement in a shorter time. On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge. Each day concluded with a short discussion where participants can express their feelings about their experience that day.

This year we shortened the School by two days by dropping the scientific excursion and the ten minute participant presentations. We had been concerned that the participants were worrying too much about preparing their presentations from midway through the School, rather than concentrating on the material we were trying to teach. While giving a short presentation is good experience, we think that it is not essential for the aim of the School. A side benefit of the shorter School is the reduced subsistence costs. We concluded that this change was beneficial and will repeat the shorter format for the next School planned for June 2019.

The questionnaire filled in by the participants provided overwhelmingly positive feedback. The perennial criticism is the intensity of the School. Participants often wish for more breaks so they can digest the content better. To do so would add accommodation costs and require more time from our team of dedicated tutors, so we feel people have to accept that it is an intense block course, unlike a semester course. 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. The personal impressions of one of the participants are given below.

We are very grateful for the generosity of the sponsors and supporters: Department of Chemistry of the University of Zürich, Swiss Society of Crystallography, Cambridge Crystallographic Data Centre, European Crystallographic Association, International Union of Crystallography, Oxford University Press, Rigaku Oxford Diffraction, Dectris Ltd, Oxford Cryosystems, Hotel Coronado, Zürich, the Chemistry Platform of the Swiss Academy of Sciences, and MiTeGen.

Tony Linden, Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2017 – Report from a participant

The Zurich crystallography school exceeded all of my expectations in terms of the quality of tutors, lectures, layout and venue. I was very impressed with the university, hotel and the convenience of the hotel being just a short walk through the park, which provided a nice place to relax in when we were able to.

Having a background in powder diffraction, I had previously not been happy with my grasp of some of the concepts of crystallography. These very difficult concepts were explained clearly and in several ways to us by the tutors. I feel so lucky to have been given the opportunity to learn from such experienced crystallographers, and having one tutor per pair of participants was incredibly beneficial to us. They all went above and beyond, very eager to answer questions at any time and spend time with participants - even late in the evening!

Since crystallography is used in so many areas of science, I was concerned about having many topics that weren't relevant. This was not the case and I ended up really learning a lot from the less relevant talks. My other main concern was about the intensity of the course, of which I was warned, however with so many breaks throughout the day and a carefully planned schedule alternating between lectures and practical sessions this wasn't a problem. The organisers clearly spent a lot of time working out the best way to arrange everything, and this made a huge difference.

The practical sessions were invaluable, especially being able to measure our own crystals on the instruments we use in our home institutions and then actually analyse this data. All the practical exercises were incredibly useful and taught us how to handle a variety of different challenges that we are likely to face. It was so enjoyable to interact with the tutors and other participants, I appreciated having a mixture of people from such different backgrounds to learn from and socialise with. Zurich is a beautiful place and we were lucky to have a day off to explore the city.

From this course I feel like I have gained knowledge of the theory of crystallography as well as all the practical aspects I need to go forward, including how to measure and solve crystal structures, which I would not have had the opportunity to learn elsewhere. This is vital for my current position as well as future career, as being taught correctly and thoroughly now will enable me to use this and pass on this knowledge in the future.

The course also gave me a greater appreciation of crystallography than I had previously, and has inspired me to consider new career paths within this area. I highly recommend this course for anyone wanting to gain a proper understanding of crystallography and learn from the best of the best!

Emily Reynolds, University of Oxford, UK