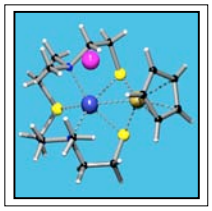
The Zürich School of Crystallography

Bring Your Own Crystals



University of Zürich

June 7 - 20, 2015

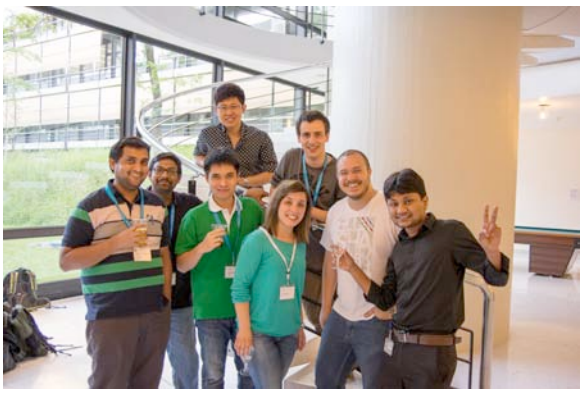
The sixth Zürich School of Crystallography was held within the Department of Chemistry at the University of Zürich (UZH). Within five minutes of the opening mixer starting, we knew the school would be an outstanding success: the 19 participants and 10 tutors were all chatting with each other enthusiastically. After 13 days of intense theory and practical sessions on all aspects of small-molecule single-crystal X-ray crystallography, the participants were still excited, although tired, and the final banquet finished with lots of book-signing by the tutors, photography and the occasional tear because new friends were going their separate ways.

We maintained our usual 2:1 student:tutor ratio and participants always comment very favourably on the personalised friendly attention they receive. The 19 participants this year comprised 1 MSc and 15 PhD students, 2 postdocs and 1 researcher from industry. They came from 12 countries: Australia, Canada, Croatia, Germany, Israel, Portugal, Russia, Slovenia, Sweden, Switzerland, Thailand and the United Arab Emirates. The 10 tutors were from the Universities of Basel, Bern, Geneva, Zürich, the EPFL Lausanne, the ETH Zürich and the Institute of Physics, Prague. This year we had two second-generation participants: PhD students whose supervisors were PhD participants themselves at one of our first schools.

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 used the Olex^2 software this year and found it to be didactically suitable in the School environment, readily understood by the participants and replete with a wide range of functionality and options.

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 participants worked on two real-case example data sets with which they learned to use the software and to recognise and resolve unexpected difficulties with structures. Each participant then determined the structure of the compound they had provided crystals of in the lead-up to the School. The 'bring your own crystal' concept is highly motivating because the participants work on the structure of a compound of specific interest to them. All these structures were completed successfully. On the final day, each participant gave a ten minute presentation on their own structure. Everyone 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. The breaks offered relaxation in the pleasant environment of the university campus. Interesting discussions with the tutors often continued over the evening meal and beyond.

The half-day excursion was to the Swiss Light Source and SINQ neutron spallation facility of the Paul Scherrer Institute. The participants are always very impressed when they see the immensity of the facilities. This year, we were able to collect data live and astonishingly quickly from one of the participant's samples at one of the SLS PX beamlines.



The questionnaire filled in by the participants provided very positive feedback about the quality of the School, the friendliness and approachability of the tutors, the organisation and the venue. Participants often say they would like a longer less intense school so they can digest the content better and wish to work on additional structures. Unfortunately this is not really feasible given the accommodation costs and the availability of the tutors, who generously donate two weeks from their hectic schedules, and to whom we are most grateful. 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. Our next School is scheduled for June, 2017.

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 Corporation, Dectris Ltd, Bruker AXS, Oxford Cryosystems, Paul Scherrer Institute, Hotel Coronado, Zürich, the Chemistry Platform

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Tony Linden, Hans-Beat Bürgi, School Directors

The Zürich School of Crystallography 2015 – Report from a participant

Given the fact that several Croatian crystallographers attended the ZSC in past years, it has a somewhat famous status among the Croatian crystallographic community. When applying for the school I had no doubt in my mind that it will be an intense course, maybe even exhausting at times, but definitely worthwhile. All of my expectations were met.

So far I have been preparing crystals and using solved crystal structures in my work, but it was always someone else doing the measurement and solving the structure for me. Due to its complexity, single crystal analysis never seemed to be an easy to master technique and even though one could use the software just by clicking the buttons and not worrying about what is all there in the black box behind, it is still not trivial and, personally, this was the only technique I always felt intimidated by. Having completed the ZSC course, I now feel confident about performing the analysis myself and I am sure I will be able to recognize and even solve problems I find on the way.

The course was a well-organized mix of lectures and tutorials given by the ten tutors, all of whom were very helpful, friendly and always ready to answer any of the student's questions. At the end of each day we had a half-hour student session where students gave their feedback on the day and could ask for repetitions or program modifications. Practical sessions involved learning on how to measure, solve and refine crystal structures. I found lectures and practical sessions to be well balanced. Also, since students came from many different fields of chemical research and had different use for solving crystal structures, I found it was very useful for all to learn through solving not only prepared example structures, but also their own structures of pre-sent crystalline compounds.

The course also included a visit to the Paul Scherrer Institute and the Swiss Light Source with a demonstration of a single crystal measurement on one of our own crystals, which allowed us to see up-close how it all works. Impressively, the measurement took only six minutes.

Apart from the lectures, the social component of the school was just wonderful. Students and tutors socialized at every breakfast, lunch break and dinner. There was also a barbecue which was a lot of fun and a great dinner party at a Chinese restaurant at the very end of the course. I thought it was wonderful to have so many different people from all around the world getting along so well and enjoying their time together.

To conclude, I think the ZSC is definitely worthwhile. In one of his review papers, Peter Müller wrote that crystallographer's training is similar to that of a Jedi Knight, where practical knowledge passes down from the master's mouth to the apprentice's ear and is not something easily learned from a textbook. I believe that ZSC with its intensity and two students per tutor ratio definitely provided the students with the most important tricks of the trade. All students need to do now is to solve structures and gain their own experience.

I really enjoyed the ZSC and I will make sure to recommend it to anyone in need of crystallographic knowledge.

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