

The Zürich School of Crystallography

Bring Your Own Crystals



University of Zürich
June 19 - 30, 2022



The 10th Zürich School of Crystallography was held as usual in the Department of Chemistry at the University of Zürich (UZH). The 20 participants (11 female) comprised one MSc and 17 PhD students, one postdoc and one research associate. They came from 14 countries: Belgium, Croatia, Finland, Germany, Greece, Italy, Morocco, Norway, Poland, Slovakia, Slovenia, Sweden, Switzerland and Zimbabwe.



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. The daily schedule is a blend of lectures, exercises and practical work, including the opportunity to gain experience at one of the five diffractometers we have available, which include dual-source Rigaku Oxford Diffraction Synergy and Supernova instruments as well as a Bruker Venture D8 diffractometer. As usual, we had our very popular 2:1 student-tutor ratio. Lively discussions between the participants and tutors also took place outside the formal class times.

All of the participants were very engaged and enthusiastic throughout the School. The levels of experience of the participants were varied, but all came away having learnt something new



and feeling better equipped to tackle their own structure determinations. Many new friendships were forged and the group was very cohesive. On the 6th day, the going got a bit tough because of a COVID-19 outbreak, three participants and three tutors tested positive and had to isolate. This necessitated implementation of hybrid sessions so that those isolating could still follow the lectures via Zoom. For the computer-based practical work this group could form their own little school in the garden of the hotel (see group photo). We are most grateful for everybody's untiring patience and willingness to pitch in and help with other organisational matters, such as delivering meals to those isolating in the hotel. The entire group handled the problems with a phantastic team spirit.

For teaching the concepts of symmetry, in addition to online materials, we break into small groups and use wooden and plastic models representing all point groups. The ability to hold and tumble such models helps the participants acquire the concepts more easily. It was also great fun watching the participants cutting their apples in the "La coupe du roi" exercise to demonstrate stereochemistry and chirality.



As an introduction to structure solution and refinement, the participants work on several example structures of varying degrees of difficulty and with different challenges. They are designed to allow the participants to see into the black box and learn about the actual procedures going on when various buttons are clicked in the software and to interpret whether or not appropriate results are obtained. Each participant then works on the data set collected from one of their own crystalline samples. We used the *Olex²* software once again for most of the structure refinement work. The ease of use of *Olex²* and the extensive range of tools and graphics that it incorporates, such as for modelling disorder, allows us to demonstrate many aspects of structure solution and refinement in a didactically beneficial way.

We no longer have a fully equipped computer classroom readily available to us because the Department of Chemistry, UZH moved to a new building. The participants therefore had to bring their own laptops and pre-install the software we planned to use. Mostly, this worked well, with only a couple of issues, usually related to an institution-supplied loaner laptop being locked against installation of new software.

Each day concluded with a short discussion where participants could express their feelings about their experience that day and we received some valuable feedback during these moments, allowing us to tweak some aspects of our sessions on the fly. On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge.



The farewell banquet is an emotional time for everyone after making so many new friends. Each participant received a certificate, Swiss chocolate and a copy of "Crystal Structure Refinement, A Crystallographer's Guide to SHELXL" by Peter Müller.

The questionnaire filled in by the participants provided very positive feedback, although it was clear that many found the programme too dense and that more breaks and personal study time need to be scheduled into the programme. We are considering extending the school by at least one day in 2024, but are mindful of the fact that this adds to the accommodation costs and time commitment required of the tutors. The personal impressions of two participants are given below.

This School presented some new challenges for the organisers. The closure of the hotel next to the UZH campus meant we had to find new accommodation and evening meals at a reasonable price, which is not trivial; the hotel we chose added 30 minutes each way to the day's travel time. This contributed to some of the questionnaire remarks about needing more time in the programme. We will try to optimise this for the next School.

While we had 39 applicants for the School, 19 of them withdrew their interest, mostly because they were unable to obtain funding for their travel and subsistence. This seems to be a common problem at the moment for similar schools, such as the ECS. Although we can distribute a few bursaries using funds kindly offered by some of our sponsors (IUCr, ECA, CCDC), we cannot usually cover the full subsistence costs, let alone travel expenses. Unfortunately, there is no student accommodation in Zurich, so we are reliant on hotels and they are not cheap in Switzerland. This limits the ability of some people to attend. For example, we had three applicants from Zimbabwe, but in the end only one very talented student could attend.

We gratefully acknowledge 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, Rigaku Oxford Diffraction, Dectris Ltd, Oxford Cryosystems, Bruker AXS, Anton Paar, Eldico Scientific, Oxford University Press, and Michael Wörle for taking many photographs, some of which are in this report.

Hans-Beat Bürgi, Tony Linden, School Directors

The Zürich School of Crystallography 2022 – reports from participants



What an amazing experience it was to participate in the Zürich School of Crystallography 2022! Ten days of being fully devoted to crystallography flew by in a moment, but even in that relatively short time, a lot of knowledge was gained, whilst at the same time priceless memories were made.

I started my crystallographic journey a few years ago when I enrolled in Ph.D. studies in a group where crystallography is a crucial research component. There I got familiar with some basic concepts, which allowed me to easily solve “routine” structures. However, during the research, I encountered a variety of advanced crystallographic problems, which required a proficient understanding of underlying principles in crystallography, especially X-ray diffraction. For those reasons, The Zürich School of Crystallography seemed like a perfect choice to help me obtain valuable knowledge that would allow me to overcome crystallographic obstacles. And that hypotheses proved to be true!

I must say that the organizers of the Zürich Crystallography School, Prof. Anthony Linden, and Prof. Hans-Beat Bürgi, did a splendid job! Even before the school started, we were provided with thorough travel and school information and material well in advance, thus making our trip to Zürich and preparations for school much easier. During the whole school, they carefully listened to participants’ impressions, wishes and needs, to determine if any improvements were needed, and to make us all satisfied with the school, thus ensuring that each one of us gets the most out of it, which is really impressive. They ensured that everything went smoothly and handled every unexpected situation promptly and effectively.

The school program was quite intense but, in my opinion, very well structured, with a good ratio of theory and practice. The first two days consisted mostly of lectures, sequentially building up from basic concepts to more advanced topics. The lectures were followed by practical sessions in groups of two or five students per tutor. I especially liked this aspect of the school, where we had a chance to discuss and resolve specific problems in detail with our tutor and obtain a further explanation of troublesome topics concerning lectures or other subjects of interest. I was very pleased that a decent amount of time was dedicated to solving structures. Starting with several example structures, we learned to treat different kinds of problems, after which we were prepared to tackle our own structures. During that time, I learned quite a lot, not only how to solve, refine and finalize the structure, but even more importantly, how to think (critically) about every step of the process and result obtained. Our tutor showed us a whole new dimension of noticing the fine details, to which I usually would not devote as much attention as needed, and these proved to be extremely informative and useful.

Another aspect that made this school unique is that we had one whole afternoon dedicated to hands-on work on the diffractometer, again in small groups of two students per tutor. We went thoroughly through the whole procedure of collecting the X-ray diffraction data, from selecting the proper crystal to setting up the measurement, with all the tips and tricks for obtaining the best possible data for a given crystal. I found this experimental session very useful, as we got a chance to ask all the specific questions concerning our usual samples and troubleshoot problems that we frequently encounter.

In the last day of school, we had an opportunity to test our knowledge by taking a two-hour written exam, which I found to be quite beneficial as I got a feeling about which parts I

should revise, and work harder on. I can conclude that participating in this school resolved a lot of questions I had and it provided a comprehensive overview of theory and practice in crystallography. I learned a lot of new things and reviewed some known concepts from a different perspective, which consequently shed new light on the way I will work in the future.

I must express a great gratitude and admiration to all tutors of the Zürich School of Crystallography 2022. Their unprecedented engagement in passing the knowledge to us through lectures and practical sessions, with passion and clarity, made me forget about the morning sleepiness. Instead, each day I got up motivated and excited to come to the University and explore new avenues of crystallography. Their unquestionable experience and the diversity of the scientific specialties they brought to this school, allowed us to get the answers to every question asked and helped us piece together some aspects of the intricate puzzle of crystallography. I find that their devotion to providing us with answers at every conceivable moment from breakfast till bedtime, readily, patiently, and relentlessly, by always finding new and creative ways to explain crystallography and challenge our knowledge in a fun and innovative way, is the true treasure of this school and its ultimate value!

And in the end, I want to express a great gratitude to Prof. Hans-Beat Bürgi and Prof. Anthony Linden for providing me with the opportunity to participate in the Zürich School of Crystallography 2022. In addition to gaining invaluable crystallographic knowledge, I met a lot of wonderful people and made new friends. All the discussions and (crystallographic and non-crystallographic) adventures we had made this school an experience I will never forget.

This school was everything I hoped for and even more! I enjoyed every single moment of it, and I would do it all over again! Thank you so much!

Mateja Pisačić, Department of Chemistry, University of Zagreb, Croatia



I recently participated in the Zurich school of crystallography from 19th-30th June, 2022 and would like to share my experience about the school. I am a PhD student at Lund University and many of the previous PhD students from our lab, who had attended this school in past years, had recommended that I participate in this summer school. For me, who was a complete beginner in the field of crystallography, it was a wonderful opportunity to get to know about the field. I had so much to learn from the school starting from the basic theory behind diffraction of waves to finally being able to mount my own crystals on the diffractometer and further solving their structure using *OLEX*². I felt that the course is a perfect combination of theory and practical knowledge and in such a short interval of time, the school managed to cover most of the relevant topics of the field. The fact that there is a tutor for every two students makes things easier to learn and it really helps a lot in understanding the concepts and to clear the doubts. The school had practical sessions with the tutors almost every day where we got to solve our own crystal structures and also deal with some practice structures using *OLEX*², which helped me a lot in getting familiar with the software. I also felt that the tutors were really giving their best to make sure everyone gets the most out of the school and they were also available outside school hours for any help. Also, the course content and material given to us both before and during the course was quite helpful. I also want to mention that the school had such an excellent social environment among the students and the tutors, which is a very important part of learning and overall, I am really happy that I got the opportunity to participate in the school.

Nitish Kumar Garg, Lund University, Sweden



I became interested in crystallography during my undergraduate studies, I measured monocrystalline inorganic materials and tried to solve their structures. My knowledge, despite attending lectures on solid state physics and studying the issues of X-ray diffraction by myself, still did not allow me to fully understand and interpret the results obtained during these experiments. I was still wondering to what extent my studies corresponded to reality and if at some point in the procedure I had not made a serious error or misconduct. As a PhD student, I found out about the Zurich School of Crystallography, and the description of the event matched what I wanted to learn. I just had to go there. I applied to school and started fundraising. Thanks to the kindness of the director of my doctoral school, my supervisor and the ECA bursary, I secured the necessary amount.

The organizers made sure that we could fully focus on learning and talking to other participants - we were provided accommodation and morning and evening meals, during the breaks between lectures, we were offered coffee, tea and sweets. It is hard to imagine better learning conditions.

Step by step, we became familiar with one crystallographic question after another (starting with the question of what a crystal is, and ending with quantum crystallography) and then we performed exercises in groups of several people under the supervision and help of one of the tutors. The exercises allowed us to learn the material on an ongoing basis.

A few days after the beginning of the course, we were formed into groups of two students, and for the rest of the school, we learned to solve and refine structures together for several hours a day under the supervision of a permanent tutor.

Another element of the course, which was particularly valuable didactically, was the possibility of measuring and solving the structure of the crystal grown by hand. We were able to compare the experimental procedures and the resolution and refinement process performed by us and by the experts on the same sample, which was the best method of identifying the errors we were making.

The course ended with an exam, thanks to which we could check the extent to which we acquired the knowledge and skills passed on to us.

I learned the stages from the formation of crystals to the publication of data, I understood the concepts necessary to be a conscious crystallographer, I learned to use methods that were unknown to me, I got answers to questions that have been bothering me for years, I met wonderful people. It made my work even more interesting and gave impetus to the implementation of new research concepts. I would like to thank the organizers and lecturers of Zurich School of Crystallography and the ECA organization as well as sponsors from my University for the opportunity to participate in the School, thanks to which I owe it all.

Pawel Butkiewicz, University of Bialystok, Poland