

# The Zürich School of Crystallography

## Bring Your Own Crystals



University of Zürich  
June 16 - 27, 2019



The 9th Zürich School of Crystallography returned from Tianjin, China, where the 8<sup>th</sup> school took place, to the Department of Chemistry at the University of Zürich (UZH). The 20 participants comprised 1 BSc, 1 MSc and 15 PhD students, 1 postdoc and 2 junior academics. They came from 13 countries: Brazil, Croatia, Finland, Germany, Greece, Hong Kong, India, Morocco, Portugal, Russia, Slovenia, Switzerland and Tunisia.



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.

(left: Lukas Palatinus lecturing on difference Fourier syntheses)

In our experience, symmetry is a notoriously difficult topic. Apart from lectures, we use tutorials with small groups of five students and one or two tutors, which has proven to be effective. (right: Tony Linden leads a tutorial on point groups)



On the third day, the students work with the crystals they brought to the school; they select a crystal, put it on one of the five diffractometers accessible at ETHZ and UZH, and measure and process a data set. The diffractometers included the modern Bruker Venture D8 and Rigaku Oxford Diffraction Synergy instruments, which are impressive in terms of speed, the availability of two radiation wavelengths and detector sensitivity. (above: Nils Trapp with students at his instrument)



In preparation for interpreting their own data, the students solve three example structures of varying degrees of difficulty. They 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 appropriate results are obtained. Each participant then works on the data set collected from their own sample.



In our fully equipped computer classroom, we used the *Olex<sup>2</sup>* software once again this year and find it to be quite suitable in the School environment. The ease of use of *Olex<sup>2</sup>* allows us to demonstrate more aspects of structure solution and refinement in a shorter time. The ever-expanding range of special tools and options in the program for easily handling special modelling issues, such as disorder, is very useful. As usual, we had our very popular 2:1 student:tutor ratio. (Céline Besnard, top front, Pascal Schouwink, middle, and Gervais Chapuis, bottom, with their students)



Each day concludes with a short discussion where participants can express their feelings about their experience that day. (right: Tony Linden and Bernd Schweizer receiving feedback)



All of the participants were very enthusiastic and maintained their eagerness and dedication throughout the School. 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. Everyone mixed well, chatted eagerly together and became friends. When the youngest participant, Liza, had her birthday midway through the school, her companion students got her cakes and candles and sang ....



On the final day, each participant sat a two-hour written exam either to obtain ECTS credit points or to self-test their knowledge.



At the end of each afternoon, after classes and feedback session are over, the day is not yet finished. Students and tutors eat dinner together and get to know each other on a more personal level. It is not unusual that the tutors are asked to clarify undigested material after the meal and sometimes deep into the night. (*left: Céline Besnard, Nils Trapp and three inquisitive students*)

Before returning home, all participants met for a Chinese 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. (*right: Tony Linden and Hans-Beat Bürgi handing out certificates and books*)



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 commitment from our team of dedicated tutors, so we feel people have to accept that it is an intense block course, unlike a semester course. The personal impressions of two participants are given below.



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*Hans-Beat Bürgi, Tony Linden, School Directors*

### **The Zürich School of Crystallography 2019 – two reports from participants**

It is an honor and pleasure to pen down my experience during ‘The Zurich School of Crystallography 2019 (ZSC)’ that has excelled in terms of the quality of teaching, tutorial sessions, layout of the course and the venue. When I started my PhD in Oct, 2016, I came to know about this school but the deadline had already passed so unfortunately, I couldn’t apply

for it. Genuinely, I felt terribly sad and since then I had been waiting for the next announcement. The wait came to an end in 2019, and has been worthwhile.

Initially I was bit concerned about the duration and the efficiency of the school as usually such long-term schools or workshops fail to stay consistent throughout the mentioned time span. This school has crossed all my expectation limits, because it was such an incredible platform for beginners in crystallography. I was amazed with the versatility of the course module including international participants with entirely different academic backgrounds. My other major concern was that, how intense is this course going to be? However, small tea/coffee breaks during the day and a carefully planned schedule have made everything absolutely effortless. There must be a delicate balance that has to be maintained to keep the participants interested and motivated till the end. Clearly, after attending the school my experience is that organizers have spent significant time working out the best way to arrange everything, and this made a huge success of ZSC-2019. The atmosphere of the university and two students per one tutor ratio were incredible. The accommodation in the hotel is just perfect as it is so convenient and relaxing to commute.

I never had a course in crystallography before, but after attending this school, I feel that I wouldn't have learnt better than this school. Having started my PhD in diffraction, I really had a hard time to understand my research problems. Actually, I lacked the vision to appreciate the beauty of symmetry and crystallography. These are somewhat difficult concepts and were thoroughly explained in several ways to us by the tutors. They all were so passionate about teaching and sharing their experiences with the participants and very eager to answer questions at any time and participating in never-ending scientific discussions with participants – even till late in the evening!

Since crystallography is a fundamental concept used almost in every scientific field, I was skeptical about the several and different topics that may happen to be irrelevant. This was not the case and I actually ended up learning a lot from all the talks. The invaluable practical sessions are at par excellence, especially one tutor per two students and being able to analyze the data from our own crystals, data that were also obtained on the instruments we use in our home institutions. To interact with the tutors and other participants and socializing with them was also great. It was so motivating and rewarding that at the end of a day, one can actually give his/her sincere opinions about the lectures and practical sessions in the form of feedback.

To conclude, from this course I feel like I have enhanced and polished my knowledge of crystallography and also how to implement this tool to tackle difficult research problems. This knowledge is crucial for my current position as well as in my future career, as being taught so thoroughly now I will be hopefully able to use this and pass on further in the near future. The course has exposed me to one of the most beautiful disciplines 'Crystallography' and taught me to appreciate crystallography. I was actually scared of it before coming here. I highly recommend this course for everyone who wants to see the world of crystallography under the guidance of pioneers of this field. Once again, I must say, hats off to the commendable job done by the organizers.



Thank you!

*Guratinder Kaur, Paul Scherrer Institute, Switzerland*

## My experience at ZSC 2019

As an organic chemist I am always faced with the uncertainty of synthesizing the correct product. And even though there are several methods which help determine what compound you prepare, I believe that having an X-ray structure of that compound indubitably confirms what you hold in your hand.

For those who wish to learn the theoretical background and gain practical experience of an X-ray experiment from the very beginning (how to grow your crystals) to the final touches at refining and publishing your structure, then the Zürich School of Crystallography is the best way to do it. Looking back at my experience I can honestly say, I would do it again and again. Even though it is an intense 10-day course covering both theory and experimental work, the amount of knowledge and level of expertise presented gives you a valuable experience that you will never forget. It is a highly interactive school, as you get the chance to work on a diffractometer, as well as gain as much theory needed to later solve your own crystal structures. An important value the school offers is being able to work, study, and debate with 10 highly experienced crystallographers, who become your tutors for the whole time in Zürich. Each tutor is assigned only two participants, which makes this school a luxurious opportunity to obtain valuable knowledge. During the school all the tutors are always available and willing to help you understand certain topics you find yourself struggling with. From my point of view, the friendliness and level of expertise of all the tutors truly places this school at the very top.

The motto of the Zürich School of Crystallography is “Bring your own crystals”, which means you are given the opportunity to send your crystals prior to your visit, so you can work on your structure once you are there. This is especially valuable for those who struggle with solving more difficult structures. Hence, having so many experts at hand can really help you understand and solve your structure.

The school is very well organized as all the lectures and exercises are carried out smoothly. Everything is prepared before you even arrive. From lecture notes, meals, coffee breaks, social events etc. Moreover, all the participants stay in one hotel near the University of Zürich, which makes it not only convenient getting to class on time, but also gives you the opportunity to socialize with other participants. To spend almost two weeks day and night with a certain group of people definitely creates new friendship bonds that will last long after you say your goodbyes.

To be given the opportunity to be a part of the 2019 Zürich School of Crystallography not only enriched my understanding on crystallography, of which I will most definitely benefit in my professional field, but also gave me the chance to meet some amazing people who made my stay truly unforgettable.



*Helena Brodnik Žugelj, University of Ljubljana, Slovenia*