Your Questions Answered

From Online Seminar:
Unlocking Efficiency: SC-XRD and APEX Software Breakthrough

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The following list is a selection of questions asked prior to and during the online seminar. If your question is not covered or has not been answered yet, please do not hesitate to contact us.

Q: How can I get access to APEX5?
A: The most easiest way of getting Access to APEX5 is buying one of our single crystal instrument. Each system comes with a lifetime site licence for APEX5. This licence can be used all over the site. APEX5 is also available through the Bruker sales channel. You can find your local sales representative through the Bruker web page on www.Brukerr.com. Of course are also happy to provide you with the contact information. Drop us a quick message through the chat window or via email.

Q: How can I get access to Cirrus? What does it cost?
A: If you have an account on www.brukersupport.com and you are registered as a user of one of our single crystal instruments the user inface shows a request button for CIRRUS next to the image of your instrument. If you press the request button you will undergo an approval process which will take a day or two. After approval you will have access to CIRRUS as a provider. As a provider you can add additional accounts for your students or for your collaboration partners. For the time being the usage of CIRRUS is free of charge. If you upload huge amount of data we might have to start charging you for the cloud service which is behind. At the moment the usage is free of charge.

Q: Why does the completeness of my data collection with different crystals systematically stuck 72 or 73% with different crystals? How can we solve the problem when planning the run strategy?
A: In principle, modern X-ray diffractometers should be able to collect data sets with a completeness of 100%. If you have a systematic problem, we needed more details to investigate the situation. However. I would be very surprised if this problem comes from a Bruker instrument.

Q: How can I solve structures with low I and high R values?
A: First of all, I means intensity, and R is the agreement factor either of the reflections with respect to each other or the agreement of the measured intensity with your crystallographic model. While I (or better I/sigma(I)) should be high, the R-factors should be as low as possible. A very straight way to improve the intensity of the diffraction signal is trying to get better quality crystals. This is often easier said than done. The second option to improve the intensity of the diffraction signal is using better instrumentation. This is in the first place moving towards stronger X-ray sources and using the most sensitive detectors such as the PHOTON III generation. Getting better crystals often is also a good approach for getting the R values down. Or of course, you need to solve the underlying crystallographic problem, such as twinning or modulation or any other crystallographic challenge you

might come across, in the first place. As Tobias has pointed out in the previous section APEX5 is highly capable to handle all these crystallographic problems. And in addition, we regularly offer trainings on the subjects to familiarise you with the crystallographic challenges. Last but not least, switching the wavelength, for example replacing molybdenum by copper radiation can also help as it also increases the diffraction signal.

Q: Do you have the CIRRUS sample submission service available in all countries?
A: Yes, we do. And we have taken care that, for example, data from our European customers are stored on European servers while data coming from our US customers are stored in facilities located in the United States and so on. That ensures that we comply with all local data safety and data privacy regulations in the various regions.

Q: How can I solve the structure if one position is occupied by more than one element.
A: Typically, this is not so much a problem of solving the structure, but more the problem of refining the structure and maybe assigning the proper element. All the refinement programs, like for example SHELXL, offer an option to refine the occupancy factor, which describes to what extend the site is occupied by a certain element. You can place multiple elements at the same position and refine the occupation factors to address this problem. Of course, the occupancy of all elements at the same position cannot be higher than one.

Q: We have already APEX5 on our single crystal machine. When will the next version become available?
A: We are releasing APEX5 updates regularly and typically we sent in announcement to all registered users through www.bukersupport.com. So, if you are registered as a Bruker user with your single crystal diffraction machine, you should receive a respective E-mail by end of next month latest. The emails will also give you a quick overview on what else has been updated.

Q: Can you get to try out version of APEX5?
A: Yes, you can. The process is very similar to getting a full licence. APEX5 is export control regulated even for temporary licenses. Therefore, get in contact with your Bruker representative, please.

Q: We had problems assigning elements.
A: This is a pretty short question lacking some basic information. The phenomenon can be caused by lacking resolution or if the overall data quality is very poor and insufficient to fully determine the structure. We are happy to assist you with this kind of problems. So, contact us in case you come across issues like that, please.

Q: Does all this work only with minerals from the database?
A: Of course not. This system as such is totally innocent of the structure you are using it for. It can cope with any crystalline structure you come across. We are searching four different databases. The first one is a local one, which is created populated with each structure measured on your local machine or with structures from all the machines in your local network. In addition, we search the COD, the CSD, and the ICSD. This covers inorganic structures, organic structures, metal organic structures. In short, almost any structure in chemistry, which ever has seen an X-ray beam.

Q: Can SC-XRD be used on Zintl phases?
A: The plain answer is yes it can.

Q: Which services used for CIRRUS?
A: CIRRUS is totally cloud-based service. Like you might have seen from manual downloads we are using Amazon cloud service to provide you with CIRRUS. We benefit from all the safety measures Amazon has established for this cloud service.