Workshop on "Problems, Errors and Pitfalls in Single Crystal Structure Analysis"

We are excited to announce that we will host this workshop at Clarkson University following the week of the 2019 annual meeting of the American Crystallographic Association.

When? August 5-8, 2019, 3.5 days, with August 4 and afternoon of August 8 being travel dates.

Where? Department of Chemistry & Biomolecular Science, Clarkson University, Potsdam, NY. Clarkson is located in upstate NY at the edge of the beautiful Adirondack Mountains.

Travel suggestions. We are easy to reach by car from the greater areas of New York, Vermont, Quebec and Ontario (e.g. 2 h SW of Montreal, QC; 2 h SE of Ottawa, ON; 2.5 h NE of Syracuse, NY; 3 h W of Burlington, VT). Nearest airports in the order of distance from Clarkson: Ogdensburg, NY (OGS), Massena, NY (MSS), Ottawa, ON (YOW), Montreal, QC (YUL), and Syracuse, NY (SYR).

About the organizers. Profs. Mario Wriedt of Clarkson University and Christian Näther of University of Kiel, Germany are the instructors. We both share a passion for crystallography with strong backgrounds in related educational and research areas. Christian offered this workshop very successfully in Kiel, Germany for many years.

Who should attend? Students, post-docs and faculty who have already gained at least some practical experience with structure determinations are invited to participate. Some basic knowledge on crystal symmetry and space groups would be welcome.

Registration fee. $300/person. This covers lodging and all instructional materials. Computers and snacks/drinks will be provided. Lodging is in newly renovated and air-conditioned dorms in double occupancy. Single room arrangements maybe be available with request. Meals are on a self-pay basis in student cafeteria or close-by restaurants.

Details and background about the content. Single crystal X-ray diffraction is one of the most common and precise methods for structure determinations. The relatively small experimental effort for a routine X-ray structure determination as well as the revolution in data processing has led to an enormous spread of this method in recent years, which means that non-experienced users can frequently perform their own structure determinations. However, sometimes problems occur that impede data collection or structure solution or yield an unusual structural model. Even if a structure seems to be successfully determined, errors might have occurred which are difficult to detect. All of these problems will be addressed at this workshop. The workshop is divided into five topics: (1) problems with the determination of the crystal system, the Laue symmetry and the space group; (2) problems with structure solution; (3) problems during structure refinement; (4) twinning and; (5) precision, accuracy and assessment of the quality of

a structure determination. Each topic will be introduced with a lecture followed by hands-on tackling of structural problems using common crystallographic computer software as described in the workshop manual. Finally, the solutions for all problems will be discussed with the whole group.

How to register? Please email Mario Wriedt (mwriedt@clarkson.edu) your name, affiliation, address and email. You will be provided a link with instructions to process the payment of the registration fee. Registration closes on May 31, 2019. The workshop is limited to 30 participants.