CRYSTALLOGRAPHY TIMES

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WELCOME

By the time you read this, summer will be over and fall will have begun. At my house, the skeletons have already started coming out from storage in preparation for Halloween. Maybe trick-or-treating will be back to normal by October 31.

To address the loss of crystallographic training opportunities resulting from the cancelation of conventional schools around the world due to the COVID-19 pandemic, Rigaku started an online crystallography school with live lectures and live Q&A using Zoom Webinar. This summer we held our fourth school, the second on advanced topics.

I would like to brag a little about the success of the Rigaku schools. *In toto*, we have had 2290 students attend at least one lecture, conferred 589 Certificates of Achievement, and reached 66 countries. This month, our video links consist of five of the most popular lectures from both the basic and advanced schools.

At the end of July, *Structural Dynamics* published our paper on the first two schools: Teaching a large-scale crystallography school with Zoom Webinar, *Struct. Dyn.* **8**, 019401 (2021). We are planning a third school on basic topics January 10-14 and 17-21, 2022 and a third advanced topics school in June of 2022. Please check here for details.

In October, we will conduct an Electron Diffraction (MicroED/3DED) Workshop on 10/27 and 10/28 from 0800 CDT to 1100 CDT. We have arranged for a group of speakers at the forefront of this exciting technique and hope you will find the workshop enlightening. You can register here.

We have a listed a few interesting crystallography articles, and Jeanette reviews *They Knew: The US Federal Government's Fifty-Year Role in Causing the Climate Crisis*.

Enjoy the fall weather,

Joe

RIGAKU'S VIRTUAL CRYSTALLOGRAPHY SCHOOLS

In this issue of *Crystallography Times*, we are providing links to five popular lectures that have been part of our schools to date. If you were unable to attend any of our schools, we hope that these lectures will be useful for enhancing your knowledge of crystallography as well as an idea of what to expect at our next school.

Rigaku Virtual Crystallography School: Non-spherical Atom Refinement with NoSpherA2

Lecturer: Florian Kleemiß

Modern diffractometers routinely produce data of quality much higher than the common model used for refinement can explain. The residual densities observed are, however, not random. They do carry chemical and structural information. In this tutorial, NoSpherA2 (Non-Spherical Atoms in Olex2) will be shown as a tool to obtain superior structural results from identical data only relying on a better model of the atomic shape. Using this technique, the routine refinement of hydrogen atom parameters becomes possible alongside improved uncertainties of all atom positions and displacement parameters. The control and interpretation of results from such refinements will be discussed and differences in comparison to spherical atom refinements highlighted.
Watch Lecture >

Rigaku Virtual Crystallography School: Data Collection Part 1

Lecturer: Pierre Le Magueres

Rigaku single crystal X-ray diffractometers all come with CrysAlis^{Pro}, a user-inspired data collection and data processing software for small molecule and protein crystallography. Designed around an easy-to-use graphical user interface, CrysAlis^{Pro} can be operated under fully automatic or manual control, allowing users different levels of intervention according to whether an easy data collection is carried out or a more problematic case must be tackled, such as a twinned crystal, a pseudo-symmetry issue in the lattice or a modulated structure.

Screening and Data collection is separated into 2 lectures. In this first lecture, we will give an overview of the most commonly used strategies to crystallize small molecules complexes. This will be followed by a live analysis of a well-diffracting small molecule crystal, using the Rigaku microfocus sealed tube X-ray diffractometer, the XtaLAB Synergy-S. We will cover crystal mounting/centering and screening/indexing. Beyond demonstrating the CrysAlis^{Pro} capabilities, tips for the best practice for each of these steps will be discussed.
Watch Lecture >

Rigaku Virtual Crystallography School: Data Collection Part 2

Lecturer: Pierre Le Magueres

In this second lecture, we will cover strategy calculation (following screening from the previous day) and data collection. We will show how concurrent data processing in CrysAlis^{Pro}and structure solution using AutoChem (an automated version of Olex2) are performed even as data collection proceeds. Lastly, a feature very unique to CrysAlis^{Pro} will be demonstrated: "What Is This". This feature allows for the collection of a fast data set to 1 Å for the purpose of getting the connectivity of a compound, as quality control for what is in the crystal when a detailed and refined crystal structure is not needed.
Watch Lecture >

Rigaku Virtual Crystallography School: PDF: What?, Why?, How?

Lecturer: Simon Bates

Atomic pair distribution functions (PDFs) have a venerable history for material structure analysis and were first applied to X-ray diffraction analysis by Debye and Menke in the 1930s. An atomic pair distribution function as measured by X-ray diffraction is essentially a histogram of atom-atom distances weighted by the electron density at each atom and is an essential component of the Debye diffraction theory. You may wonder why any of that should be of interest to you. But it turns out that one of the best ways to collect X-ray data suitable for PDF determination is using a single crystal diffraction system, and there are many materials problems that can only be addressed by using PDF methods. In this session we will learn more about the elegant beauty of PDFs and the Debye diffraction theory, how we collect optimum data and the type of analysis that can be performed.
Watch Lecture >

Rigaku Virtual Crystallography School: Twinning

Lecturer: Fraser White

Twinning is a commonly encountered phenomenon in X-ray crystallography which can make life more difficult. It is highly likely that you will encounter twinning in your crystallographic career if you have not already. Modern software and better hardware have made treatment of twinning much more routine however understanding what twinning is and how it can be handled is still important knowledge for a crystallographer to ensure the best results can be achieved. This session will therefore explain the different types of twinning which can occur, their traits and thus how to identify them, and the circumstances under which they might arise. Following this, strategies for treating twinned samples, from data collection and processing through to structure solution and refinement will be discussed.
Watch Lecture >

BOOK REVIEW

They Knew: The US Federal Government's Fifty-Year Role in Causing the Climate Crisis
By James Gustave Speth
ISBN: 9780262542982

They Knew is not like most books about the climate crisis. Despite the presentation of its publication as a book, it is in fact a copy of James Gustave "Gus" Speth's expert testimony in the case *Juliana vs. the United States*. In 2015, 21 youth plaintiffs filed a lawsuit against the United States claiming government officials had violated their unalienable rights to life and liberty by pursuing a national agenda in support of fossil fuel consumption, despite having extensive knowledge regarding the negative and inevitable impact of such behaviors on the (near) future climate of the planet.

The case is still ongoing. As of the writing of this review, the plaintiffs are in the middle of settlement negotiations. However, despite the frequent legalese in the introduction, written by Julia Olsen and Philip Gregory, the two adult litigators leading the plaintiffs' case, the rest of the book is much more rooted in history and the science of those historical times. You do not need to be a lawyer to parse the majority of the book, although the introduction definitely tests the reader's basic knowledge of legal terminology.

Speth's book is divided into nine chapters, prefaced by an introduction in which he explains his *pro bono* role as an expert providing testimony on behalf of the plaintiffs in *Juliana*. He also clarifies that, although this testimony was originally written and published in 2018, he reviewed, revised, and updated it in 2020 to include the full impact of the most recent administration.

In the first chapter, he lays the groundwork for what the United States government knew about climate change at the beginning of the Carter administration. The following seven chapters are broken out by presidential administration, from Carter through Trump. In each chapter, Speth outlines both the advances in understanding of climate science during that president's term and how the policies they enacted and supported impacted the well-being of the environment at that time. No administration comes out of Speth's testimony entirely spotless, although perhaps the worst offender is the most recent one, from 2017-2020. Under Trump's presidency, almost all previously enacted climate protections were undone, and any progress made during previous administrations was entirely lost. The full list, provided in bullet form for ease of reading, is indeed still difficult to digest.

The final chapter contains Speth's damning conclusion—as the title of the book suggests, "they knew" (the "they" in question being the United States government) how the actions and policies enacted by the various administrations of the past 40 plus years would negatively impact future generations. But Speth keeps his testimony very factual, leaning on evidence from verifiable sources such as recorded speeches and official documentation. He doesn't try to posit why these decisions were made, only that they were, despite the mounting scientific evidence they would have dire consequences in the near future.

The book ends with an appendix written by Olsen and Gregory, updating the reader as to the status of *Juliana* as of the time of the book's publication.

The last hundred or so pages contain Speth's extensive references, as well as a note confirming his professional background, as it qualifies him to provide testimony in *Juliana*.

They Knew is not a fun, light, or entertaining summer read, but it certainly casts a bright and educational light on a dark history of covering up climate change.

Jeanette S. Ferrara, MFA

RIGAKU TOPIQ WEBINARS

Rigaku has developed a series of 20–30 minute webinars that cover a broad range of topics in the fields of X-ray diffraction, X-ray fluorescence and X-ray imaging. You can register here and also watch recordings if you cannot attend live sessions.

CRYSTALLOGRAPHY IN THE NEWS

August 23, 2021: Researchers in the UK and Germany have synthesized and characterized a tri-nuclear thorium complex with a Th-Th aromatic l-bond.

August 27, 2021: Brändén and Neutze provide a review on the advances and challenges in time-resolved macromolecular crystallography.

September 15, 2021: Researchers in the US suggest a mechanism for the entry of the Hepatitis C virus into the host cell via acidification and receptor binding prior to membrane fusion.

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Our LinkedIn group shares information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories. You can also catch up on the latest newsletter or *Rigaku Journal* issue. We also hope that you will share information about your own research and laboratory groups.

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RIGAKU X-RAY FORUM

At rigakuxrayforum.com you can find discussions about software, general crystallography issues and more. It's also the place to download the latest version of Rigaku Oxford Diffraction's CrysAlis^{Pro} software for single crystal data processing.

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9009 New Trails Drive, The Woodlands, TX 77381, United States