Rigaku

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WELCOME

It has been a busy month. Abstracts for oral presentations were due May 17 for IUCr and May 23 for ACA. I hope you have or will have met the appropriate deadline by the time you read this message. Having said this, I know that both the ACA and IUCr have been working hard to plan meetings with excellent scientific content and the best in virtual networking. Here are the ACA meeting web page and the IUCr meeting page. I look forward to seeing you at both meetings.

We have a rather long list of webinars this month, with topics including MicroED, pharmaceutical analyses, the Rigaku School for Crystallography, an Asia-Pacific Users' Meeting, diffuse scattering and high-pressure crystallography.

Rigaku has announced two awards in honor of esteemed crystallographers we lost in 2020: Ed Stevens and Ward Smith. These awards are open to graduate students or postdoctoral fellows who have exhibited excellence in their crystallographic-related research and meet the criteria of either of the two awards as described below.

In this issue, we highlight Professor Makoto Fujita's crystalline sponge method as practiced on a Synergy diffractometer. We also place Professor Chris Hill of the University of Utah in the spotlight. You will also find our usual roundup of useful links and videos. Finally, Jeanette reviews a book on the interactions of trees among themselves.

All the best,

Joe

RIGAKU CRYSTALLOGRAPHIC AWARDS

The Ed Stevens Award for Excellence in Small Molecule Crystallographic Research

Ed Stevens was an early pioneer in charge density analysis, or what is now known as "quantum crystallography." He was a highly productive researcher throughout his career and helped develop many aspects of the science, including appropriate treatment of thermal diffuse scattering, accurate data collection at liquid helium temperature, error estimation of charge density maps, measurement of diffraction intensities at absolute scale, treating anharmonic motion, and the use of scattering factors based on wave functions, to name a few.

The winner of this award will be someone who has demonstrated an ability to push the envelope in the field of small molecule crystallography to further our understanding of structural science.

The Ward Smith Award for Excellence in Macromolecular Crystallographic Research

Ward Smith spent most of his career in industry. He started at Monsanto in St. Louis working as a structural biologist, then moved to Agouron Pharmaceuticals in San Diego at the beginning of structure-based drug design. He then joined SmithKline Beecham in Philadelphia. He ended his career as a program director of the National Institute of General Medical Sciences (NIGMS) where, among other things, he managed the Protein Structure Initiative and the NIH-sponsored synchrotron beamline facilities.

The winner of this award will be someone who has demonstrated an ability to perform ground-breaking research utilizing macromolecular crystallography to enhance the future of mankind.

The winner of each award will receive a plaque and a cash gift of $1000. Graduate students or postdoctoral fellows apply here.

CRYSTALLOGRAPHY IN THE NEWS

April 13, 2021: Researchers in China and the U.S. report the packing of a supramolecular truncated cuboctahedron into double-helical nanowires on a graphite surface with a non-natural parastichy pattern.

April 22, 2021: Researchers in the U.K. and U.S. have synthesized and characterized a MOF that can store ammonia at 293 K at a density almost the same as solid ammonia at 193 K.

April 26, 2021: Researchers from UCLA and Yale have determined the correct structure of (–)-lomaiviticin C using microcrystal electron diffraction ending two decades of deed-end syntheses.

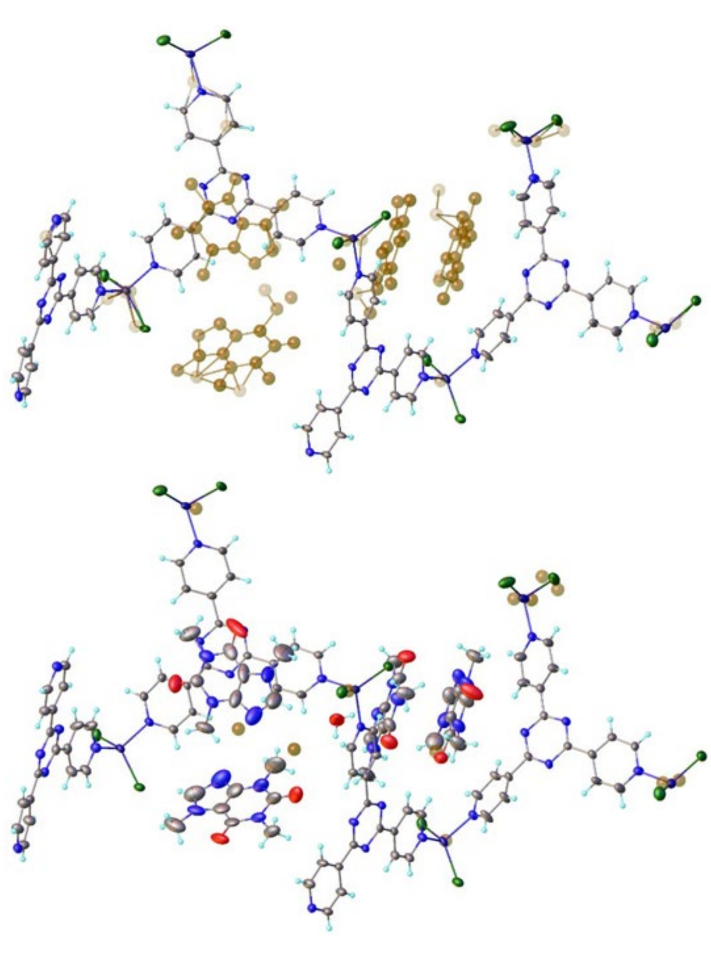
April 28, 2021: Scientists at the University of Erlangen-Nürnberg have synthesized and characterized a series of strongly reducing Mg(0) complexes.

May 7, 2021: A large group of scientists from Europe and the U.S. have used X-ray screening of 2381 compounds to identify the active site and 37 allosteric inhibitors of SARS-CoV-2 main protease.

May 14, 2021: Researchers in the U.K. and U.S. have determined that the chain of chirality in Te nanocrystals is determined by screw dislocation during formation.

WHAT CAN YOU DO WITH YOUR SYNERGY?

The Crystalline Sponge Method



Crystal structure of caffeine inside a crystalline sponge. The guest molecules are clearly visible in the difference electron density map.

The Crystalline Sponge (CS) method is an approach to obtain single crystal X-ray structures of compounds that are difficult or impossible to crystallize; for example, because they are of too small a quantity, are not solid at ambient conditions or form amorphous precipitates. In some cases, spectroscopic or spectrometric techniques cannot give definitive answers to the analytical problems, so a crystal structure is needed. The CS method utilizes a metal-organic framework (MOF) as a host for analyte molecules (guests). Analytes can diffuse into the pores of the MOF from solution or the gas phase and align themselves in an ordered fashion, which is predetermined by binding sites of the MOF cavity. This induced-fit molecular recognition process can be understood as crystallization inside a crystal.

A new application note from Rigaku shows an example of a Crystalline Sponge measurement from start to finish. Caffeine was chosen as an appropriate guest molecule for the CS method because it is a representative example of a small molecule active pharmaceutical ingredient (API). $ZnCl_2$-based CS crystals were prepared according to literature described procedures. A single crystal was transferred to a conical shaped vial, along with 50 μL cyclohexane and 1 μL caffeine solution (1 μg/μL in CH_2Cl_2). The vial was closed with a screw cap equipped with a PTFE liner. The liner was pierced with a needle and the solvent was allowed to evaporate at 50°C over the course of two days. Diffraction data was collected using Cu-Kα radiation on a XtaLAB Synergy-S (Cu, Mo) and a HyPix-6000HE hybrid photon counting detector at 100 K. In total, 1862 frames were collected, with exposure times of 0.24 s and 4.40 s, giving a total experiment time of 1:34 hours.

READ APPLICATION NOTE

RESEARCHER IN THE SPOTLIGHT

Christopher P. Hill
H.A. and Edna Benning Endowed Chair
Distinguished Professor, Biochemistry
Vice Dean of Research for the School of Medicine

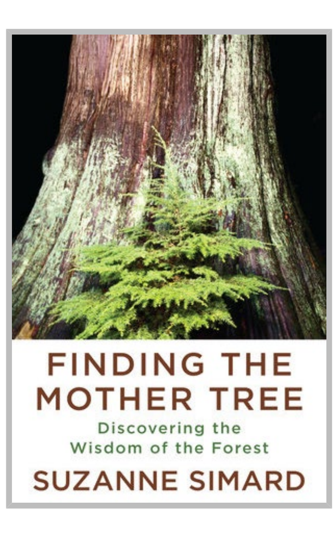
University of Utah
Department of Biochemistry

The Hill Group seeks to understand mechanisms of biology at the level of structures, interactions, and conformational changes of protein molecules and their interacting partners. They study multiple biological pathways and questions using a variety of approaches, especially electron cryo-microscopy (cryo-EM), X-ray crystallography and biochemistry. They collaborate extensively with colleagues that use complementary approaches, including genetics, genomics, cell biology and animal models.

Their current projects include HIV-host interactions, AAA protein translocases, D-peptide therapeutics, chromatin regulation, insulin therapeutics and the ubiquitin-proteasome system.

For the HIV-host interactions research project, they are partners in the HIV P50 HIV structural biology consortium – CHEETAH (Center for the Structural Biology of Cellular Host Elements in Egress, Trafficking, and Assembly of HIV). Their interests and contributions include architectural components of the virion and cellular factors that either counteract the virus or are recruited to facilitate viral replication.

BOOK REVIEW



Finding the Mother Tree: Discovering the Wisdom of the Forest
By Suzanne Simard
ISBN: 978-0525656098

Suzanne Simard's *Finding the Mother Tree* is a *Silent Spring* for the next generation. Just as Rachel Carson's groundbreaking work illuminated the negative environmental impacts of DDT, so does Simard's book provide readers with an unprecedented glimpse into the lives, minds, and cultures of forests.

Finding the Mother Tree, like *Silent Spring*, is masterfully written. Dressed in the garb of a memoir, the book is just as much about Simard as it is about her work, but in such a way that serves to underscore her dedication to her research, rather than draw focus away from it. Simard carefully weaves her interpersonal narrative of memories with her hyper-focused academic one, providing readers with a book that makes learning about the complex neural networks of trees seem somehow easy, even though the concept is mind-blowing.

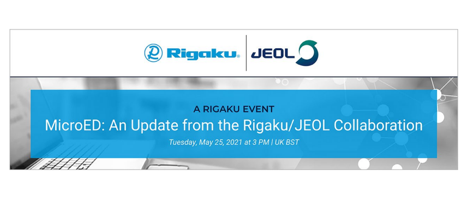
A wonderful read as we ease from spring into summer, after devouring *Finding the Mother Tree,* one may find themselves never really looking at forests the same way again.

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.

UPCOMING EVENTS



We would like to invite you to join us for a special webinar on MicroED. During this event we will show you the latest progress from our collaboration with JEOL.

Presenter: Fraser White
Date/time (CDT): Tuesday, May 25, 2021 - 09:00 AM
Time Zone Converter

REGISTER

Pharmalytical Summit 2021 is a one-day educational experience focused on the technology, research, and innovation that go into developing pharmaceuticals to help people live longer, healthy lives.

The day features presentations and discussions with industry leaders and experts who will share their knowledge and expertise in order to help bring these life-changing products into the world. Join us for a day of education and insights for the pharma professional related to the drug development lifecycle. The day is designed around four tracks: Discovery, Pre-formulation, Formulation, and Manufacturing & Control. There are breakout sessions throughout the day, as well as main event sessions including a roundtable discussion of polymorphs in pharma. This event is focused on the United States but welcomes participants globally.

Hosted by Chris Carolan
Date/time (CDT):
Wednesday, May 26, 2021 - 08:00 PM
Time Zone Converter

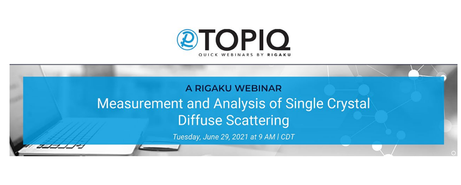
REGISTER

You are invited to a series of 10 tuition-free, hour-and-a-half webinars on advanced topics in practical X-ray crystallography.

We will cover microED, Olex2, Twinning, the Cambridge Structural Database, powder data collection and processing, Pair Distribution Function (PDF), Small Angle X-ray Scattering (SAXS), protein crystallography, non-spherical atom refinement with NoSpherA2 and charge density.

The series runs June 7–18, 2021 at 8:00 AM CDT every weekday.
Time Zone Converter

REGISTER



Diffuse scattering is a continuous signal that is present between Bragg peaks. It is especially prominent in disordered crystals and, if modeled, allows us to understand the real structure of such crystals at local scale.

In this workshop, we will introduce the concept of diffuse scattering, show how to measure it, and how to analyze it using a fast method based on the three-dimensional difference pair distribution function. We will start from the basics and do not expect from participants any prior knowledge on diffuse scattering or disorder modeling.

Presenter: Dr. Arkadiy Simonov
Date/time (CDT): Tuesday, June 29, 2021 - 09:00 AM
Time Zone Converter

REGISTER

We would like to invite you to join us for our single crystal users' meeting, held online via Zoom. The meeting will take place at 2:00–5:00 PM JST on both days to allow our users from the Asia Pacific region to attend.

Date/time (CDT) - Session 1: Tuesday, June 29, 2021 - 11:00 PM
Date/Time (CDT) - Session 2: Wednesday, June 30, 2021 - 11:00 PM
Time Zone Converter

REGISTER

This workshop is primarily geared towards crystallographers with little or no experience in high-pressure crystallography and who are interested in learning how to get started. Presentations are intended to be practical and educational and will include reviews of diamond anvil cells (DACs) and accessories from two DAC manufacturers, sample preparation under pressure in DACs, sample mounting/centering on a Rigaku diffractometer and data collection, and data processing and correction. The workshop will be held on July 21–22, 2021 at 8:00 AM CDT.

Date/time (CDT) - Session 1: Wednesday, July 21, 2021 - 08:00 AM
Date/Time (CDT) - Session 2: Thursday, July 22, 2021 - 08:00 AM
Time Zone Converter

REGISTER

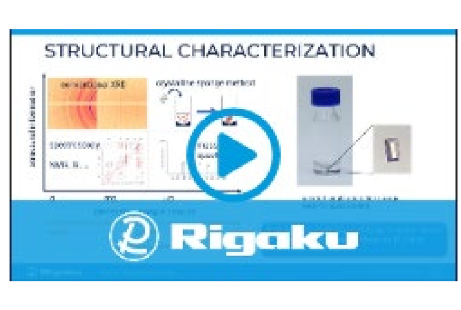
RIGAKU REAGENTS

Custom Stock Solution Library:

Rigaku Reagents can help you build your own customized solution library and never run out of a stock solution. These stock solutions are ideal for systematic grid-screening of initial crystallization hits. Select the stock solutions you use from our buffers, salts, polymers and precipitants, or let Rigaku Reagents know what type of solution, container, volume or label you need and we'll prepare it for you. This will allow you to immediately follow up on any crystallization hit and maximize reproducibility with consistent quality of sterile stock solutions. Contact ReagentOrders@Rigaku.com for more information or visit us here.

SHOP HERE

VIDEOS OF THE MONTH



Rigaku TOPIQ: Crystalline Sponge Method

The Crystalline Sponge Method is an option to obtain structural information for compounds that are otherwise inaccessible to common crystallographic approaches because they are of low availability, liquids or gases at room temperature. Such sponges are porous crystalline metal organic frameworks that can absorb and orient organic molecules in their defined pores. An introduction to the method is given including a structure refinement using Olex².

Smart and Programmable Sponges from Design and Synthesis to Implementation Webinar
Dr. Omar Farha, Associate Professor of Chemistry at Northwestern University,

MOFs are a class of porous, crystalline materials composed of metal-based nodes and organic ligands that self-assemble into multi-dimensional lattices. In contrast to conventional porous materials such as zeolites and activated carbon, an abundantly diverse set of molecular building blocks allows for the realization of MOFs with a broad range of properties. The Farha group has developed an extensive understanding of how the physical architecture and chemical properties of MOFs affect material performance in applications such as catalytic activity for chemical warfare agent detoxification.

USEFUL LINKS

Crystalline Sponges as a Sensitive and Fast Method for Metabolite Identification: Application to Gemfibrozil and its Phase I and II Metabolites

https://dmd.aspetjournals.org/content/48/7/587

Metal-Organic Framework

(MOF) Constructor

Metal-Organic Frameworks (MOFs) are a novel class of 3D networked, crystalline materials composed of metal ions or clusters connected by organic linkers. Given their porous nature and often high surface areas, MOFs can be used in a variety of applications such as gas adsorption, storage, separations, catalysis, sensors, drug delivery and more.
This MOF Constructor Tool offers easy access to Millipore Sigma's portfolio of organic linkers and metal precursors including inorganic secondary building units (SBUs) suitable for the preparation of MOFs. Explore the MOF constructor tool to further learn about the properties and applications of different MOFs, including Basolite® MOFs.

JOIN US ON LINKEDIN

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.

JOIN HERE

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.

JOIN HERE

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