



Volume 13, No. 4, April 2021

WELCOME

A couple of weeks ago, we held a Virtual Users' Meeting with attendance in excess of 100 people. In-person Users' Meetings tend to be much smaller in size because of the expense and the time it takes to travel to and from the location. Zoom has made it possible for many more people from many different locations to participate in and contribute to meetings, to the benefit of all. This is exciting and portends enhanced collaboration in the future.

Speaking of meetings, we learned late last month that the IUCr Congress will either be a hybrid or fully virtual meeting. I did look forward to going to Prague and seeing old friends, but I don't think I will get to travel there. I suggest you register at the [IUCr conference website](#) and answer their questions about attendance. This will help the organizers with planning the conference.

At the end of May we have a webinar on the collaboration between Rigaku and JEOL on electron diffraction. The webpage for the June Rigaku School for Practical Crystallography is also live, and you can register for any or all days now.

In this month's "What Can You Do with Your Synergy," we'll look at collecting high-pressure data. The "Researcher in the Spotlight" is Prof. Kristin M. Hutchins from Texas Tech University. The Useful Links highlight the work of the Coronavirus Structural Task Force and a review on high-pressure crystallography by Andrzej Katrusiak. The Videos of the Month focus on high-pressure crystallography as well. Finally, Jeanette reviews Walter Isaacson's *The Code Breaker: Jennifer Doudna, Gene Editing, and the Future of the Human Race*.

All the best,

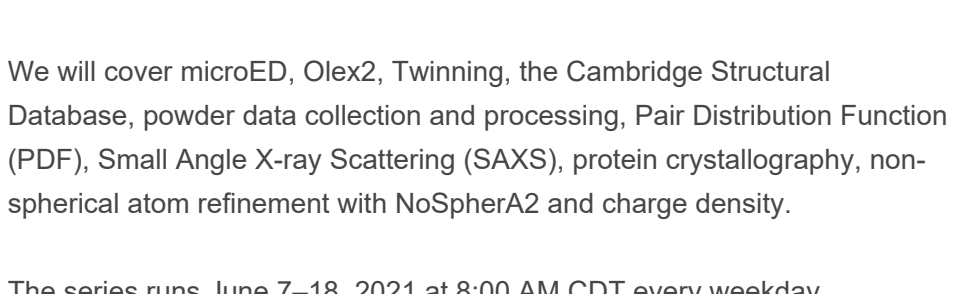
Joe

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.

[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.

[REGISTER](#)

CRYSTALLOGRAPHY IN THE NEWS

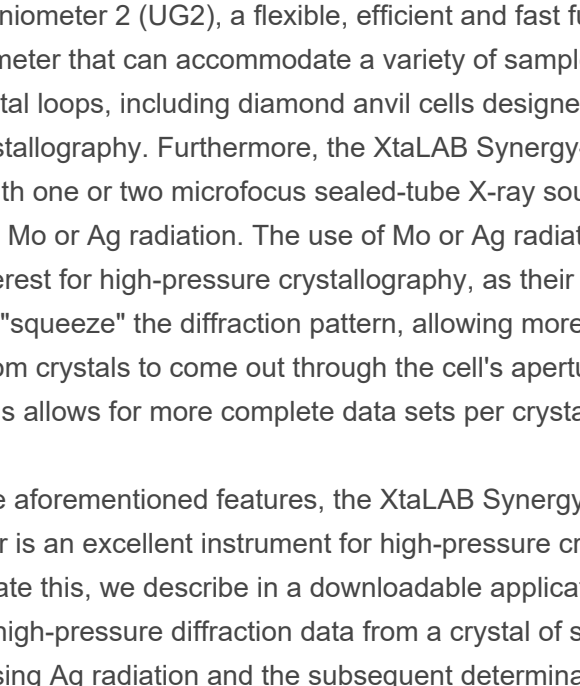
March 15, 2021: Researchers in Belgium, China and the U.S. used various methods, including powder XRD and PDF, to study LiNiB deintercalation to develop **two dimensional borides**, which have potential for novel materials.

April 2, 2021: Researchers in Germany, Italy, U.K. and U.S. used **two existing drug libraries and high-throughput X-ray screening** to find two binding sites as targets for inhibition of the SARS-CoV-2 main protease.

April 15, 2021: Scientists in Germany, Japan, Russia and the U.S. studied the electronic properties of **single crystals of κ -(BEDT-TTF) $_2$ Cu $_2$ (CN) $_3$** at various temperatures using ESR and found a spin gap at 6 K.

WHAT CAN YOU DO WITH YOUR SYNERGY?

High-Pressure Data Collection



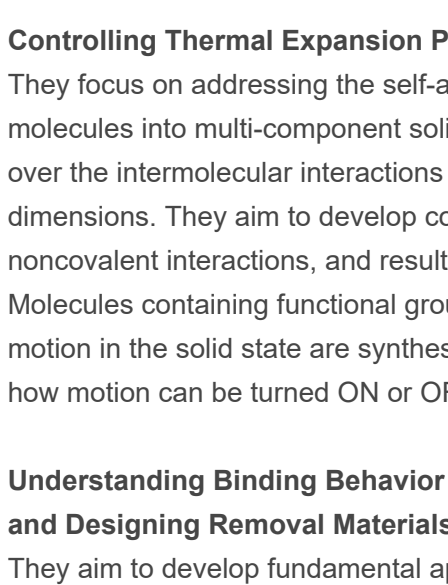
The Rigaku XtaLAB Synergy-S X-ray diffractometer is built around the Universal Goniometer 2 (UG2), a flexible, efficient and fast full 4-circle kappa goniometer that can accommodate a variety of sample holders in lieu of single crystal loops, including diamond anvil cells designed for high-pressure crystallography. Furthermore, the XtaLAB Synergy-S may be configured with one or two microfocus sealed-tube X-ray sources with a choice of Cu, Mo or Ag radiation. The use of Mo or Ag radiation is of particular interest for high-pressure crystallography, as their short wavelengths "squeeze" the diffraction pattern, allowing more diffraction reflections from crystals to come out through the cell's aperture and be collected. This allows for more complete data sets per crystal.

Thanks to the aforementioned features, the XtaLAB Synergy-S diffractometer is an excellent instrument for high-pressure crystallography. To demonstrate this, we describe in a downloadable application note the collection of high-pressure diffraction data from a crystal of sodium uranyl triperoxide using Ag radiation and the subsequent determination of its crystal structure, which led to an excellent final R1 of 3.66% to 0.65 Å.

[READ MORE](#)

RESEARCHER IN THE SPOTLIGHT

Kristin M. Hutchins
Assistant Professor of Chemistry
Department of Chemistry and Biochemistry
Texas Tech University



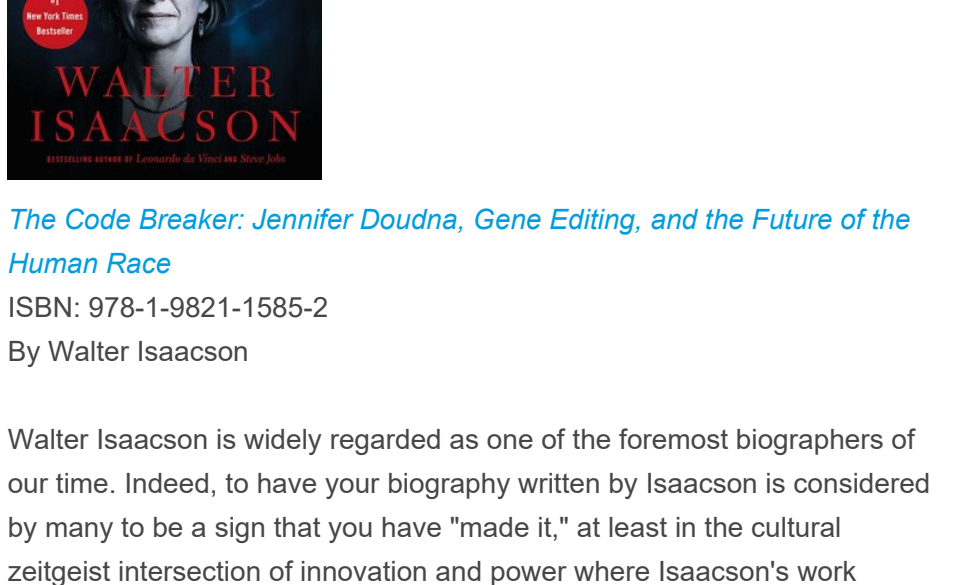
Crystal Engineering and Organic Materials

Research in the Hutchins group is inspired by the way in which nature utilizes reversible, non-covalent interactions such as hydrogen bonding and metal coordination to create large, functional structures (e.g. DNA double helix, hemoglobin).

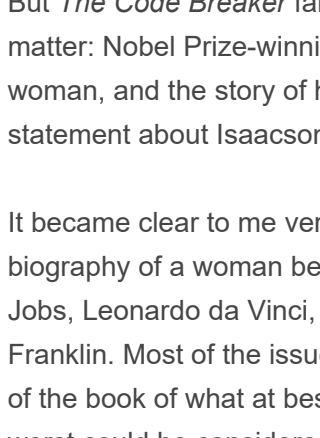
Students in the Hutchins group gain skills in molecular design, organic and polymer synthesis, and a variety of diffraction, imaging and spectroscopic characterization techniques. The group focuses on two main research areas:

Controlling Thermal Expansion Properties in Organic Materials: They focus on addressing the self-assembly of individual organic molecules into multi-component solids (e.g. salts, co-crystals) with control over the intermolecular interactions that sustain the solid in multiple dimensions. They aim to develop correlations between structure, noncovalent interactions, and resulting thermal expansion properties. Molecules containing functional groups that are capable of undergoing motion in the solid state are synthesized and characterized to understand how motion can be turned ON or OFF in a controlled manner.

Understanding Binding Behavior of Pharmaceutical Contaminants and Designing Removal Materials: They aim to develop fundamental approaches for designing and synthesizing porous macromolecular materials that will engage in reliable, noncovalent interactions with pharmaceutical contaminants. The project focuses on constructing materials designed to bind contaminants through specific, directional interactions. The project emphasizes use of small-molecule studies in the solid and solution states as a way to select the functional groups that will comprise the porous material.



BOOK REVIEW



The Code Breaker: Jennifer Doudna, Gene Editing, and the Future of the Human Race

ISBN: 978-1-9821-1585-2

By Walter Isaacson

Walter Isaacson is widely regarded as one of the foremost biographers of our time. Indeed, to have your biography written by Isaacson is considered by many to be a sign that you have "made it," at least in the cultural zeitgeist intersection of innovation and power where Isaacson's work dwells.

But *The Code Breaker* falls flat. It is not a statement about the subject matter: Nobel Prize-winning chemist Jennifer Doudna is a fascinating woman, and the story of her work with CRISPR even more so. It is a statement about Isaacson's biography of her.

It became clear to me very early on that Isaacson had never written a biography of a woman before. He is most famous for his works on Steve Jobs, Leonardo da Vinci, Henry Kissinger, Albert Einstein, and Benjamin Franklin. Most of the issues are subtle, a deep thread woven in the subtext of the book of what at best could be considered tone deafness and at worst could be considered something much more insidious.

There have been a lot of parallels made—both in the book and in society at large—between Jennifer Doudna and Rosalind Franklin. Franklin, many feel, was robbed of recognition for the Nobel Prize awarded to Watson, Crick and Wilkins for the discovery of the structure of DNA. Others disagree, claiming that Franklin, despite taking the X-ray diffraction image that led to the double helical discovery, would not have been able to figure out the structure—an unfair projection at best, a misogynistic one at worst. We'll never know what could have been or would have been, but making such comparisons in the wrong way creates uncomfortable insinuations. Suggesting Doudna's being awarded the prize was in some way a "correction" of past wrongs or a consolation prize decades in the making for a wronged Franklin both undermines the significance of Doudna's contribution and creates a problematic illusion that the men who contributed to CRISPR (and, subsequently, DNA) somehow made greater contributions than the women. It's a muddled mess, and Isaacson does a terrible job of teasing apart these intricate subtleties, especially given the controversy at the center of the CRISPR patent battle.

Isaacson also repeatedly underscores that Doudna is incredibly competitive. This in and of itself is not bad—he claims Doudna herself acknowledges her own character and the impact it has had on her work, sometimes for better and sometimes for worse. But he places a lot of emphasis on the negative impact—such as the deterioration of her relationship with Emmanuelle Charpentier, with whom she shares her Nobel Prize. It is out of place and uncomfortable in the context in which it is presented—as a recurring theme of Doudna's character—a highly competitive person, whose competitiveness is described as a flaw of her character. By comparison, Isaacson discusses Eric Lander, the head of the Broad Institute who was funding Doudna's male competitors in a recent patent battle over using the CRISPR technology in humans. Lander, who Isaacson alludes to having a, if not personal, genuinely jovial relationship with, is also described as being highly competitive but its cloaked in language of endearment and a tone of congenial collegiality. The contrast between how the competitiveness of a man who is not the subject of the book and who is not a scientist who actually worked on CRISPR is portrayed and the woman who is the subject of the book and won the Nobel prize for her role in discovering and developing the technology, is hard to ignore, and makes reading the book a less than enjoyable experience.

If you want a more gripping book about the story of CRISPR, I would recommend *Editing Humanity* by Kevin Davies [reviewed here in 2020]. If you want a better biography of Doudna, you may have to wait until a new biographer dethrones Isaacson as the historically accurate tale-teller of our time.

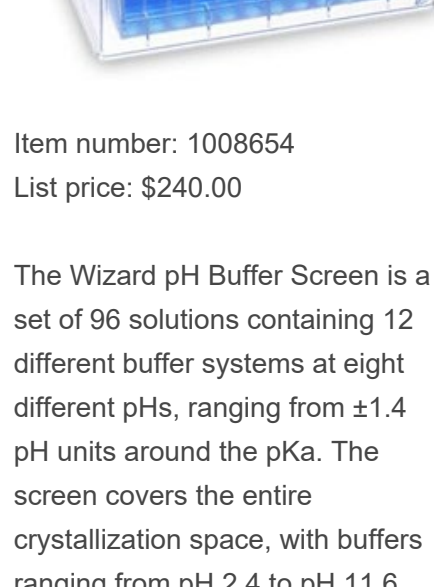
Jeanette S. Ferrara, MFA

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.

RIGAKU REAGENTS

Wizard pH Buffer Screen:



Item number: 1008654

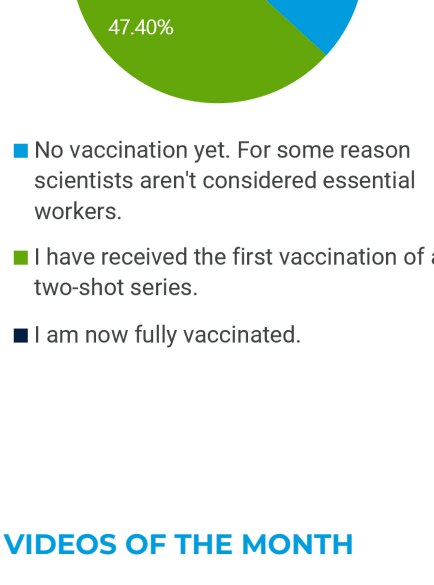
List price: \$240.00

The Wizard pH Buffer Screen is a set of 96 solutions containing 12 different buffer systems at eight different pHs, ranging from ±1.4 pH units around the pKa. The screen covers the entire crystallization space, with buffers ranging from pH 2.4 to pH 11.6. This set of buffers is designed to complement the use of any of our 96 formulation crystallization screens and can be employed to add another dimension to the search for optimal protein crystallization hits to simultaneously explore the effects of pH and buffer composition on crystal growth.

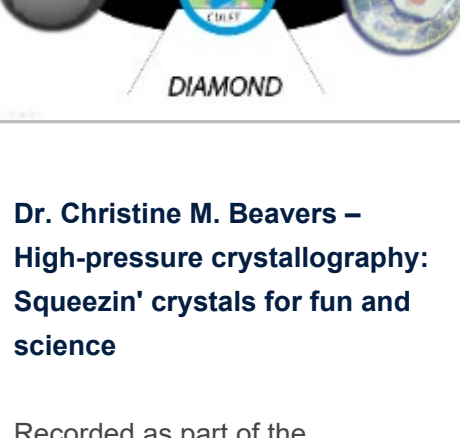
[SHOP HERE](#)

LAST ISSUE'S SURVEY RESULTS

As the COVID-19 vaccines are rolled out around the world, we are curious as to how many scientists have received a vaccination.

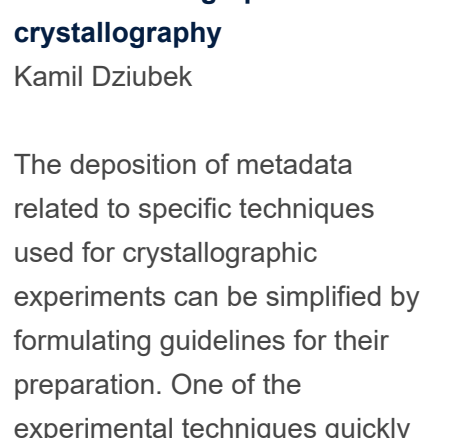


VIDEOS OF THE MONTH



Dr. Christine M. Beavers – High-pressure crystallography: Squeezin' crystals for fun and science

Recorded as part of the [#theLightStuff](#) online lecture series, Dr. Christine Beavers from the Diamond Light Source elaborates on high-pressure crystallography.



Metadata in high-pressure crystallography

Kamil Dziubek

The deposition of metadata related to specific techniques used for crystallographic experiments can be simplified by formulating guidelines for their preparation. One of the experimental techniques quickly gaining ground in the field of crystallographic research is high-pressure diffraction studies. They involve additional equipment for pressure generation, pressure calibration, etc. The high-pressure cell can interfere with the primary or diffracted beam, which can contaminate the diffraction patterns and introduce errors in reflection intensities. The experimental details are vital for the evaluation and analysis of the data, and therefore the metadata are needed to be stored along with the raw diffraction images.

USEFUL LINKS

An [international group of scientists led by Andrea Thorn](#) of the University of Hamburg has been diligently working to correct structures of SARS-CoV-2-related depositions in the Protein Data Bank to ensure scientists have the best possible structures with which to work.

[High-Pressure Crystallography](#) Downloadable article on high-pressure crystallography.

Andrzej Katrusiak
Adam Mickiewicz University

JOIN US ON LINKEDIN

Our [LinkedIn](#) forum 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 general discussions about issues, general crystallography software and more. It's also the place to download the latest version of Rigaku Oxford Diffraction's CrysAlisPro software for single crystal data processing.

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