



Volume 12, No. 8, October 2020

WELCOME

As you can see, we've redesigned our newsletter to make for a more enjoyable reading experience while still letting us keep you updated on our latest news and provide you with vital information in the crystallography field of study. We hope you enjoy the new layout.

It's been quite a month. Emmanuelle Charpentier and Jennifer Doudna were awarded the 2020 Nobel Prize in Chemistry for their pioneering work on CRISPR-CAS9. Another woman, Andrea Ghez, shared the Nobel in Physics for the discovery of black holes. All in all, a good year for women in science.

Also notable this week, an article in *Nature* suggesting that superconductivity had been observed at a balmy 15°C in a system consisting of S, C and H. This is exciting, even though this was observed in a diamond anvil cell at 2.6 million atmospheres.

In other news, **SWISSCI** is now a distributor of Rigaku Reagents screens, chemicals, and tools for Europe.

We have decided to hold an Advanced Topics in Practical Crystallography lecture series December 7–11, 2020. We will cover Powder and PDF Data Collection and Processing, High Pressure Cell Data Collection and Processing, Using Ewald3D, and Non-spherical Atom Refinement with NoSpherA2.

[REGISTER](#)

This month we spotlight the XtalLAB Synergy-R and the Northwestern University Integrated Molecular Structure Education and Research Center. You'll also find some very useful links and interesting videos below. We have two short book reviews, the first on the newest Carl Hiassen novel and the latter on a memoir by Ruth Bader Ginsburg. Finally, our survey question reflects the worldwide increase in the number of COVID-19 cases.

Stay positive and test negative,

Joe Ferrara

CRYSTALLOGRAPHY IN THE NEWS

July 6, 2020: Janssen Research & Development, LLC has joined the [Industrial Macromolecular Crystallography Association](#) (IMCA) to enhance its structural biology research programs.

September 14, 2020: Researchers in Canada and Germany have discovered a [method for one-pot, room-temperature conversion of dinitrogen to ammonium chloride](#) using boron chemistry that could lead to more efficient production of fertilizers.

September 17, 2020: Scientists in the U.S. have determined the [structure of 5-HT2A serotonin receptor with LSD bound](#). This research is part of a broader program for drug development for neuropsychiatric disorders.

October 12, 2020: Scientists at CalTech, HHMI and Rockefeller University determined the structures of eight [COVID-19 human neutralizing antibodies in complex with SARS-CoV-2 spike trimer or the ACE2 receptor-binding domain](#) in order to better develop therapeutic strategies.

October 14, 2020: Researchers at Intel, UNLV and the University of Rochester have seen evidence of [superconductivity at room temperature](#) at 267 gigapascals in a sulfur, carbon, and hydrogen phase.

October 16, 2020: Scientists at Indiana University, Northwestern University, University of Chicago and Roosevelt University have [synthesized and characterized a stable Fe\(VI\) complex](#) as a model for oxidation in biological systems.

PRODUCT IN THE SPOTLIGHT

XtalLAB Synergy-R



HIGH-FLUX ROTATING ANODE X-RAY DIFFRACTOMETER

A Powerful and Fast System for Single Crystal X-ray Diffraction Analysis

The XtalLAB Synergy-R single crystal X-ray diffractometer was designed to address the increasing need to investigate smaller and smaller samples in crystallographic research. Tightly integrating a PhotonJet-R microfocus rotating anode X-ray source with a high-speed kappa goniometer and a solid state pixel array HPC detector creates a single crystal diffractometer that produces up to 10-times the flux as compared to a PhotonJet-S microfocus sealed tube source. The increase in flux allows you to look at much smaller crystals than ever before and as an additional benefit, it provides increased data collection speed for normal sized crystals. The system can be equipped with your choice of HPC hybrid photon counting detectors, the HyPix-6000HE or the curved, large theta coverage HyPix-Arc 150°.

BENEFITS

- **Faster, accurate data collection** due to high-speed kappa goniometer, high-flux rotating anode X-ray source, fast, low-noise X-ray detector and highly optimized instrument control software.
- **Improve your ability to investigate small samples** due to the increased flux from the rotating anode X-ray source, as well as the extremely low-noise of the HyPix X-ray detectors. Noise-free images mean you can count longer for weakly diffracting crystals without a loss in data quality arising from detector noise.
- **Highest level of user safety** with multiply redundant electromechanical safety circuits built into the ergonomically designed radiation enclosure.
- **Minimize your downtime** by utilizing built-in online diagnostics and troubleshooting to diagnose and fix almost all problems without a site visit.
- **Increased data collection speed** due to the increased flux of the X-ray source.
- **Enhance your ability to resolve large unit cells, twins or incommensurate lattices** when you select the optional motorized variable beam slit in order to alter divergence to adapt the source to your sample's requirements.

LAB IN THE SPOTLIGHT



Dr. Christos D. Malliakas
Northwestern University **IMSERC**
IMSERC Associate Director,
Crystallography Director
Research Associate Professor

Professor Malliakas' research projects focus on the structural characterization of layered distorted chalcogenide materials that possess usually incommensurate modulated superstructures. He uses a variety of non-classical scattering characterization techniques like multidimensional (superspace) crystallography and Pair Distribution Function Analysis (PDF).

The Northwestern University (NU) Integrated Molecular Structure Education and Research Center (IMSERC) was established to educate NU students and researchers to be scientific leaders, support world-class research and provide access to and education for students on the use of a variety of analytical instrumentation and methodologies. IMSERC's mission is to support research throughout all of Northwestern and beyond in the areas of (but not limited to) molecular characterization, drug discovery, materials science, environmental research, translational medical research, nanotechnology, chemical biology, catalysis, pharmacokinetics, clinical research and molecular imaging. To accomplish this, IMSERC is a one-stop-shop, open-access facility that provides and maintains a suite of state-of-the-art analytical instrumentation, including single crystal and powder X-ray diffractometers, nuclear magnetic resonance spectrometers (solid state, cryo and liquid with multidimensional experiments available), gas and liquid chromatographs with UV and mass spectrometric detection (high-resolution accurate mass and nominal mass instruments capable of anything from validated quantitative methodology to untargeted screening) and physical characterization instrumentation (elemental analyses, thermal analyses, size exclusion chromatography of polymers).

The Crystallography Facility supports Northwestern Research and external users by performing solid-phase, single crystal and powder analyses on a variety of samples such as drug candidates, catalysts, organic or inorganic LEDs and energy storage networks. IMSERC's crystallography staff provide service work and offer training to qualified researchers to solve their own structures and/or collect their own data.

USEFUL LINKS

[Crystallography Open Database](#)

Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals, excluding biopolymers.

Including data and software from CrystalEye, developed by Nick Day at the department of Chemistry, the University of Cambridge under supervision of Peter Murray-Rust.

All data on this site have been placed in the public domain by the contributors. Currently there are **463229** entries in the COD.

[DECOR—The Database of Educational Crystallographic Online Resources](#)

DECOR is an online resource for the sharing and borrowing of educational resources for crystallography. The DECOR project provides a forum where crystallographic educators share resources for teaching crystallography, and where anyone who wishes to teach a course in crystallography or pursue an informal education in the art of crystal structure determination may have access to teaching resources. Use of materials on the DECOR website is absolutely free. There is only one condition to the use of materials on this site: since individuals have committed many hours of time to the development of these resources, appropriate citations for the use of these materials in the class room should be provided, and authors of the available resources should be credited.

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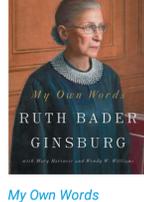
BOOK REVIEWS



Squeeze Me
by Carl Hiassen, Alfred A. Knopf, New York City, 2020, 352 pages
ISBN-13 : 978-1524733452

When I saw that Carl Hiassen had published a new book, I purchased a copy immediately and put it at the top of my queue. I did not know about you, but I needed a good, therapeutic laugh. *Squeeze Me* did not disappoint. I don't want to give away any spoilers so you can experience the joy of laughing out loud as I did. As usual, Hiassen focuses on a specific environmental issue centered within or around Florida and builds a humorous story around it. The story begins with the disappearance of a wealthy West Palm Beach socialite at a country club owned by the President of the United States. As the story progresses, Hiassen touches on current social issues, including the pandemic and immigration.

Hiassen has written a number of other novels of the same genre, as well as a handful of children's books. Be forewarned, this novel is not of the latter type.



My Own Words
by Ruth Bader Ginsburg, Simon & Schuster, New York City, 2016, 400 pages
ISBN-13 : 978-1501145247

I have to admit I had not paid much attention to the life of Ruth Bader Ginsburg until very recently. When she passed away last month, I decided it was time to fill that void and read something about her life and work. This memoir covers both her early years and her entire career in law up to the end of the 2016 U.S. Supreme Court term. Some of the content comes from her husband, Martin, but the majority is either autobiographical or derived from notable orations, including many bench announcements. RBG discusses her time on the faculty at Columbia and Rutgers Schools of Law, her advocacy for the ACLU's Women's Right Project, her time as an appellate court judge and, ultimately, her friendship with Associate Justice of the Supreme Court of the United States. Her friendship with Antonin Scalia is prominent and makes the reader wish for the time when people of different political views would listen to and respect the other's perspective without necessarily agreeing to it. This memoir taught me how vital RBG was in the fight for women's rights in the U.S. She is the first woman and the first Jewish person to lie in state in the U.S. Capitol Rotunda, a fitting tribute to a life devoted to the betterment of the U.S.

RIGAKU TOPIQ WEBINARS

Rigaku has developed a series of short, 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.

X-RAY COMPUTED TOMOGRAPHY FOR MATERIALS AND LIFE SCIENCE 7: LIFE SCIENCE APPLICATIONS

A 3D look at the structures of a reptile, insects and a mouse, including their stained organs. In the most recent episode of the webinar series "X-ray Computed tomography for Materials & Life Science," we discussed how to deal with unique challenges in life science sample preparation and introduce some quantitative analyses. You can watch the recording of it [here](#).

RIGAKU REAGENTS: Wizard pH Buffer Screen



The Wizard pH Buffer Screen is a set of 96 solutions containing 12 different buffer systems at eight different pHs, ranging ± 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.

[ORDER HERE](#)

SURVEY OF THE MONTH

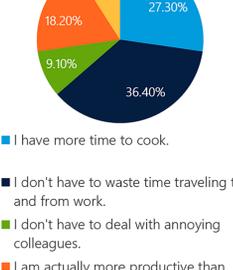
COVID-19 cases are again rising around the world in what appears to be a second wave. How will this impact your current work regimen?



[TAKE THE SURVEY](#)

LAST ISSUE'S SURVEY RESULTS

Which do you think is the most annoying thing to happen during a Zoom meeting?



- I have more time to cook.
- I don't have to waste time traveling to and from work.
- I don't have to deal with annoying colleagues.
- I am actually more productive than before.
- Nobody realizes I'm sleeping later.

VIDEOS OF THE MONTH



Early-Stage Cancer Detection with a Lanthanide-Based Metal Organic Framework

Researchers from Nankai University and the Collaborative Innovation Center of Chemical Science and Engineering in Tianjin, China, demonstrate a luminescent sensor based on a lanthanide metal-organic framework (Ln-MOF) for early detection of cancer.



David J. Haas, part 1: Cryo-cooling Protein Crystals: The First 52 Years

Dr. David Haas shares the story behind his invention of macromolecular cryo-crystallography. In his postdoctoral studies, David Haas set out to reduce radiation damage to protein crystals during X-ray crystallography. In 1970, he published a paper on his invention of macromolecular cryo-crystallography—freezing crystals to extend their lifetime in the X-ray beam. The widespread use of the synchrotron beginning in the 1970s made cryo-cooling essential, and today nearly all protein crystal structures deposited in the international Protein Data Bank use this method.

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.

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