

Crystallography Newsletter
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Come visit us at:

ACA 2020, 70th Annual Meeting
of the American Crystallographic
Association, San Diego, CA,
August 2-7, 2020.
<https://www.acameeting.com/>



Rigaku Oxford Diffraction Webinar

May 6, 2020 | 0900 CDT

Sample Screening, Strategy Calculation, and Data Collection in CrysAlis^{Pro} will be presented by Pierre Le Magueres. He will review best practices to mount/center a crystal, screen it and index it, calculate a data collection strategy and run data collection.

You may register [here](#).

A RIGAKU EVENT
Rigaku School for Practical
Crystallography

[REGISTER NOW](#)

A lot of younger members of the scientific community will be missing out on some opportunities to learn crystallography at schools and conferences this summer, so you are invited to a series of ten tuition-free 1-hour webinars on practical aspects of X-ray crystallography. The majority of the time will be spent on small molecule crystallography, but we will also air sessions on macromolecular crystallography and powder diffraction.

This is a great opportunity for people who are interested in crystallography to gain a basic foundation of single crystal analysis from a practical point of view. Please forward this information to anyone you think might benefit from such a virtual school.

Crystallography in the News

March 25, 2020: SGC PX and Diamond I04-1 released 68 crystal structures of the SARS-CoV-2 main protease in complex with putative inhibitors as part of a Pan-Dataset Density Analysis (PanDDA) group deposition. This is in addition to the 7 released on March 11.

March 25, 2020: Researchers at MIT have isolated and characterized an elusive tri-tert-butyl phosphatetrahedrane.

March 30, 2020: Researchers at Tsinghua University and the Shanghai Synchrotron Radiation Facility determined the [crystal structure of the SARS-CoV-2 spike receptor-binding domain bound to the ACE2 receptor](#).

April 3, 2020: Researchers at Scripps and HKU-Pasteur Pole have determined the crystal structure of a neutralizing antibody previously isolated from a convalescent SARS patient in complex with the [receptor-binding domain of the SARS-CoV-2 spike protein](#), providing molecular insight into antibody recognition of SARS-CoV-2.

April 3, 2020: Researchers in Canada, the UK and the US used crystallography to study allosteric poly(ADP-ribose) polymerase-1 retention on DNA breaks and [suggest an improved pro-retention compound to kill cancer cells](#).

Rigaku Reagents: JCSG Crystallization Screen Series

The Joint Center for Structural Genomics formatted the JCSG Core Suite screens as a result of analyzing over 500,000 high-throughput crystallization experiments, performed at the JCSG. The 384 crystallization formulations were selected based on the highest hit rates in initial screening.



The Wizard JCSG+™ 96 well block plate sparse matrix protein crystallization screen is designed for coarse screening of initial crystallization and solubility conditions for biological macromolecules. Researchers from the Joint Center for Structural Genomics (JCSG) formulated this screen with the goal of maximizing the coverage of the crystallization parameter space (buffers, salts, precipitants and pH) and eliminating redundancy. The buffers give final solution pHs between 4.2 and 10.5. Precipitants include volatile reagents such as ethanol, high molecular weight polymers such as PEG-8000, and salts such as ammonium sulfate.

Order Here

April 3, 2020: A group of researchers from the China, Germany, Lithuania and the US used grazing incidence XRD to [study changes in magnetic properties of perovskite manganate membranes](#) on polymer films.

April 3, 2020: Researchers in France have engineered a [polyethylene terephthalate \(PET\) hydrolase that depolymerizes PET](#) at 90% or better in 10 hours.

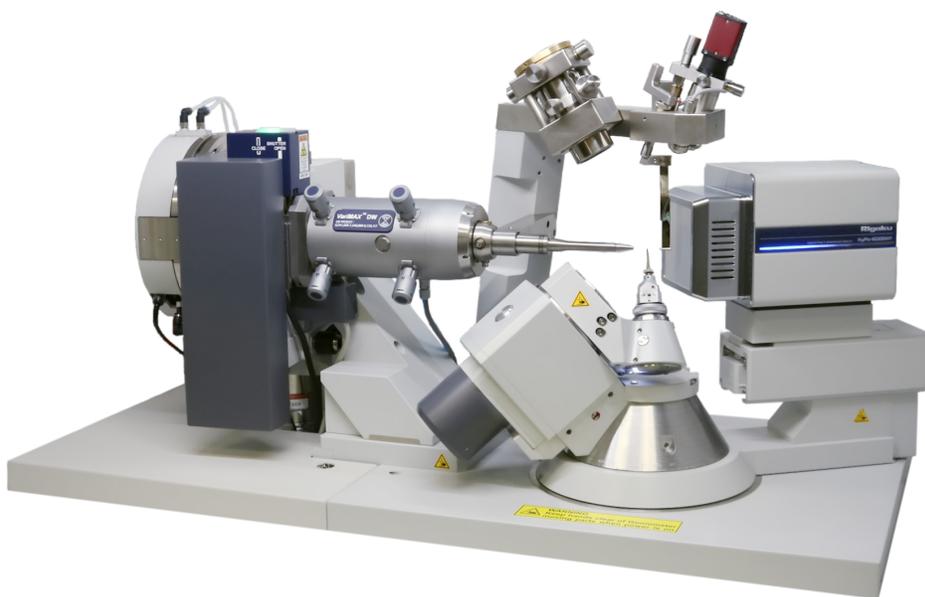
April 9, 2020: Researchers in Austria, Germany and the Netherlands have [developed direct band-gap semiconductors, capable of efficient light emission](#), from hexagonal Ge and GeSi crystals.

April 15, 2020: Researchers in Australia, Germany, Australia and the US used the LCLS to find that dense-environment effects can [strongly affect local radiation damage-induced structural dynamics on protein nanocrystals](#).

Product Introduction

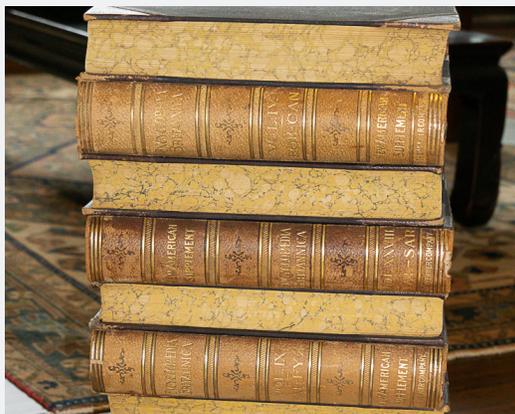
Rigaku Oxford Diffraction [XtaLAB Synergy-DW VHF](#)

The introduction in 2004 of the Oxford Diffraction Gemini diffractometer, with two independent X-ray sources, was a watershed moment in crystallographic instrumentation. The groundbreaking design of the Gemini suddenly gave crystallographers the ability to easily switch between Cu and Mo wavelengths and greatly expanded the experimental flexibility available for analyzing single crystal samples. The **XtaLAB Synergy-DW VHF** is an extension of that revolutionary idea which retains the flexibility of the dual wavelength capability but in addition adds the exceptional flux enhancement of a reliable, rotating anode X-ray source.



Survey of the Month

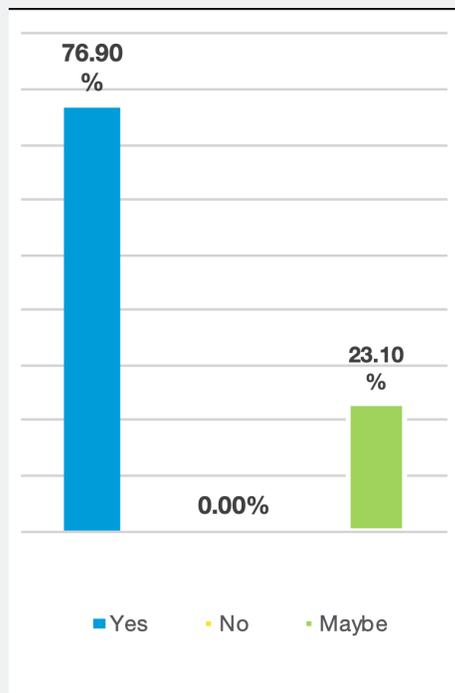
With all the children now being homeschooled, we wanted to find how they were doing:



Take the Survey

Last Issue's Survey Results

The novel coronavirus will impact climate change in a positive way by replacing face-to-face interactions with telepresence



The XtaLAB Synergy-DW VHF provides 50% more flux at the sample position over the previous DW model due to newly designed confocal optics. The ability to configure it with two different wavelengths means that with a Cu/Mo anode, the XtaLAB Synergy-DW VHF is the perfect instrument to share between structural biology and chemical crystallography groups. During times of tight resources, the sharing of instrumentation is a useful goal so that everyone can achieve success in their research.

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.
- Enhanced **experimental versatility** with two switchable wavelengths (the following combinations are available: Mo/Cu, Cu/Cr, Cu/Co, Cu/Ag, and Ag/Mo).
- Improve your ability to **investigate small samples** due to the increased flux from the rotating anode X-ray source as well as the extreme 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.

Lab in the Spotlight

Wilson Laboratory

The Scripps Research Institute

Crystallographic Studies of Immune Recognition and Viral Pathogens



The main focus of the Wilson Lab is on immune recognition and on how pathogens are recognized by the adaptive and innate immune systems. Their major goals are to understand the interaction and neutralization of foreign antigens by the immune system through structural studies using mainly high-resolution X-ray crystallography. The information

derived from these studies is being used to develop antigens and immunization regimens to elicit broadly neutralizing antibodies against viral pathogens, such as influenza virus and HIV-1.

Videos of the Month

US Navy Admiral William H. McRaven, one of the most decorated US commanders, delivers one of the best motivational speeches you will ever hear.



Watch the Video

The next outbreak? We're not ready | Bill Gates
April 3, 2015

If anyone deserves to say "I told you so" it might be Bill Gates - but I doubt if he would say that. This video was released 5 years ago and it turns out to be very prophetic.



Watch the Video

A PDB search of "Wilson, I.A." shows 5 structures deposited by this highly productive group this month alone (as of 4/20/20):

6NHP Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin HA2 I45T mutant

Wu, N.C., Lee, J.M., Thompson, A.J., Su, W., Xie, J., Lerner, R.A., Yen, H.L., Paulson, J.C., Bloom, J.D., Wilson, I.A.

6NHQ Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin HA2 I45M mutant

Wu, N.C., Lee, J.M., Thompson, A.J., Su, W., Xie, J., Lerner, R.A., Yen, H.L., Paulson, J.C., Bloom, J.D., Wilson, I.A.

6NHR Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin HA2 I45F mutant

Wu, N.C., Lee, J.M., Thompson, A.J., Su, W., Xie, J., Lerner, R.A., Yen, H.L., Paulson, J.C., Bloom, J.D., Wilson, I.A.

6O00 Crystal structure of bovine Fab NC-Cow1

Stanfield, R.L., Berndsen, Z.T., Huang, R., Sok, D., Warner, G., Torres, J.L., Burton, D.R., Ward, A.B., Wilson, I.A., Smider, V.V.

6OPA Crystal structure of bovine Fab NC-Cow1 in complex with HIV-1 BG505 SOSIP.664, and human Fabs 35022 and PGT128

Stanfield, R.L., Berndsen, Z.T., Huang, R., Sok, D., Warner, G., Torres, J.L., Burton, D.R., Ward, A.B., Wilson, I.A., Smider, V.V.

Useful Links



Best Practices for Securing Your Zoom Meetings

Since so many of us are Zooming around the world I thought [this](#) link would be useful in terms of providing better security for your Zoom meetings.



Chocolate for breakfast

For all you chocolate-loving jet-setters and shift-workers here is an article destined for a huge number of citations or an IgNobel.

Book Review



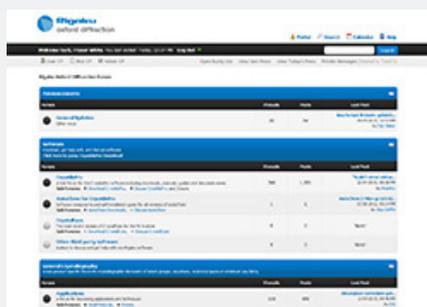
**What Stars
Are Made Of**
The Life of Cecilia Payne-Gaposchkin

What Stars Are Made Of: The Life of Cecilia Payne-Gaposchkin
ISBN: 9780674237377

Donovan Moore's *What Stars Are Made Of* paints a delightful portrait of a pioneering yet largely unrecognized astronomer whose work uncovering the composition of stars redefined our understanding of these gaseous giants.

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.



Rigaku X-ray Forum

www.RigakuXrayForum.com

Here 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.



Subscribe to Rigaku eNewsletters

Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on X-ray crystallography.

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Cecilia Payne-Gaposchkin was a true trailblazer for women in the fields of astronomy and astrophysics. She was not only the first woman to receive a doctoral degree in Astronomy from Radcliffe College, but the first woman promoted to a full-time professorial position at Harvard University. She was also the first woman ever appointed as a Harvard department head.

However, Payne-Gaposchkin's story is not well-recorded—indeed, Moore confesses in the introduction his own motivation for writing the book. A friend was auditing an introductory astronomy class at Princeton University, “The Universe.” Payne-Gaposchkin and her work made an appearance in the lecture notes. When Moore's friend shared the notes with him, Moore found himself questioning who this woman was and why he had never heard of her before. The ensuing line of questioning burgeoned into a full-blown biographical research project.

Moore tells Payne-Gaposchkin's story as fully as he can—in some spots, confessing his only evidence comes from newspaper clippings of the time. He begins with her childhood in Britain, then follows her through her young academic years, her expulsion from one school, and subsequent tenure at another, all leading up to her time as an undergraduate at Cambridge, where she studied under the likes of Neils Bohr and Ernest Rutherford. Despite the distinct “boy's club” atmosphere of the university at the time, Payne-Gaposchkin excelled in her schooling and garnered herself a post at the Harvard University Observatory following her pseudo-graduation from Cambridge (women at the time were insultingly granted degrees in title only, and not the actual physical degree itself).

Payne-Gaposchkin started a new life in America, working her way up through the hierarchy at the Harvard Observatory and earning her PhD from Radcliffe. She eventually became an American citizen, married, had several children, and continued to work. During World War II, when many home childcare providers began work in factories to support the war effort and make a better living financially, Payne-Gaposchkin even brought her children to work—and the head of the observatory essentially told her coworkers to deal with it—she was too important and her work too critical for her to stay home.

What Stars Are Made Of is Moore's biographical debut. His decades of experience as a journalist serve him well—the biography is both well-researched and well-written in accessible yet elegant prose. His lack of technical expertise is evident, but almost unnoticeable, given how compelling his portrayal of Payne-Gaposchkin's. The book is not so much about Cecilia's actual research and the exact empirical nature of her contributions to the field, but rather about Cecilia herself. *What Stars Are Made Of* is a perfect read for anyone and everyone intrigued by those historical figures marked by the passionate pursuit of scientific inquiry.



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