



CRYSTALLOGRAPHY TIMES

Volume 14, No. 11, November 2022

WELCOME

I think we all breathed a sigh of relief when we learned the two missiles of Russian manufacture that landed in Poland were fired from Ukraine. I am happy that cool heads prevailed and WWII did not start. This gives something to be thankful for.

By the time you read this, many in the US will be celebrating the Thanksgiving holidays. There is a lot to be thankful for, in addition to the item mentioned above, including a return to pre-COVID normalcy. About the only places where masks are still required are medical facilities, which, when you think about it, should have been a rule since the confirmation of the germ theory of disease.

Thanksgiving used to mark the beginning of the Christmas season in the US. I've seen decorations out in the stores since before Halloween and on houses in my neighborhood since last week. I find the refrain from Bing Crosby's "The Secret of Christmas" appropriate:

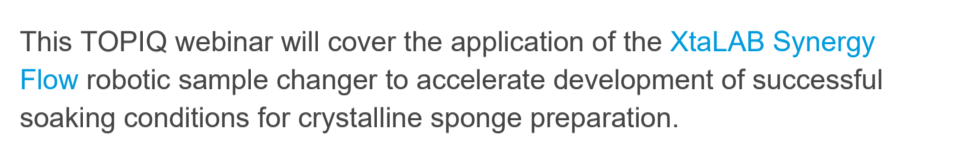
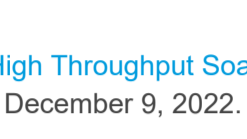
"So, may I suggest the secret of Christmas
It's not the things you do at Christmas time
But the Christmas things you do all year through"

This month we highlight two recent XtaLAB Synergy installations in Brazil, at the labs of Carlos Pinheiro, U. Federal de Minas Gerais, and Javier Ellena, Structural Crystallography Multi-User Laboratory in São Carlos, as well as highlighting the XtaLAB Synergy-S system itself.

We have two meetings and a TOPIQ webinar on the calendar for December. We hope to see you at one of these events. We continue to provide a list of Ukraine support groups in the useful links section. I also included a link to pictures from the JWST that show an exoplanet orbiting its sun. I wonder who is looking at us. Lastly, we have a few Crystallography in the News articles and Jeanette reviews *What If?* 2.

All the best,
Joe Ferrara

UPCOMING WEBINAR



Christian Göb will present [High Throughput Soaking Condition Screening For Crystalline Sponges](#) on December 9, 2022.

This TOPIQ webinar will cover the application of the XtaLAB Synergy Flow robotic sample changer to accelerate development of successful soaking conditions for crystalline sponge preparation.

The crystalline sponge method requires sponges to be placed into a solution of a target analyte so that the analyte may be absorbed by the sponge, also known as soaking. Successful soaking depends on factors such as concentration and temperature. Normally, a range of conditions might be attempted and for each an X-ray diffraction experiment is performed. The XtaLAB Synergy Flow can increase throughput by allowing batches of soaked sponges to be screened automatically and unattended to determine which conditions were the most successful.

RESEARCHERS IN THE SPOTLIGHT



Carlos Pinheiro
U. Federal de Minas Gerais

The Laboratory of Crystallography of the Federal University of Minas Gerais (LabCri), located in the Department of Physics, is a laboratory that has its origins in the early 1970s, when a diffractometer for polycrystals, Rigaku Geigerflex with Bragg-Brentano geometry and with the possibility of using radiation from Cr, Fe, Co, Cu, Mo and Ag tubes, was acquired. The acquisition of this equipment had a great impact on the quality and quantity of experimental work carried out in the material science field at the Departments of Physics, Chemistry and Geology of the Federal University of Minas Gerais and continues in operation until the present day. In the early 1990s, LabCri's experimental infrastructure was expanded with the acquisition of a 4-circle diffractometer for structural studies using single crystal diffraction techniques. In 2009, the LabCri received a Gemini diffractometer with the option of using Mo or Cu radiation and measurement temperatures ranging from 90 K up to 1000 K. In 2022, LabCri received a XtaLAB Synergy-S diffractometer with the option of using Mo or Cu radiation and measurement between 90 K and 500 K. Currently LabCri is one of the best-equipped X-ray diffraction laboratories in Brazil and keeps its doors open to researchers from different universities, research institutions and private companies from all over Brazil.

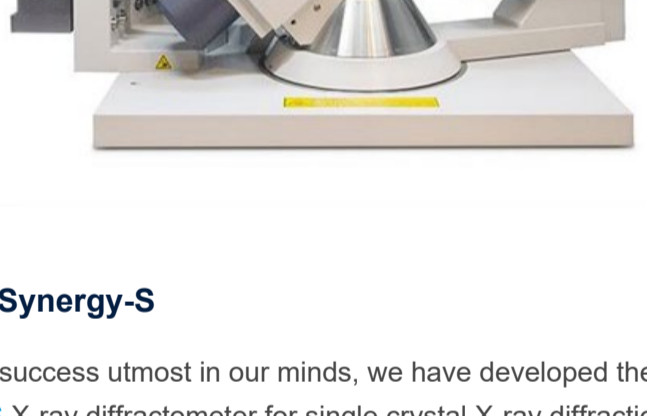


Javier Ellena
Structural Crystallography Multi-User Laboratory

The Structural Crystallography Multi-User Laboratory (LaMuCrEs) in the São Carlos Institute of Physics was the first crystallography laboratory in Brazil, originating in the 1960s with research in material sciences developed by Professor Yvonne Mascarenhas. Since then, it has supported science and technology in Brazil and South America, contributing to the formation of a cadre of Brazilian students and researchers in crystallography. The multidisciplinary character of the group enabled the development of research in different fields, mainly in the elucidation of crystal and molecular structures and the evaluation of physicochemical properties of small molecules, resulting in partnerships with laboratories from different parts of the world.

LaMuCrEs is currently coordinated by Professor Javier Ellena, an experienced researcher in crystallography who has published more than 450 papers, in addition to patents, book chapters and other materials. Ellena's group is interested in synthesizing new solid forms for active pharmaceutical ingredients, characterization of coordination compounds with biological properties and identification of Brazilian minerals.

INSTRUMENT IN THE SPOTLIGHT



XtaLAB Synergy-S

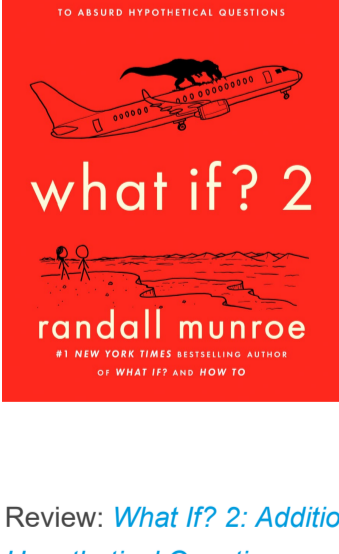
With your success utmost in our minds, we have developed the XtaLAB Synergy-S X-ray diffractometer for single crystal X-ray diffraction. Using a together of leading-edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S produces fast, accurate data in an intelligent fashion. The system is based around the PhotonJet-S series of microfocuss X-ray sources that optionally incorporate continuously variable divergence slits. These third-generation sources have been designed to maximize X-ray photons at the sample by using a combination of new optics, new longer-life tubes and an improved alignment system. PhotonJet-S sources are available in Cu, Mo or Ag wavelengths in either a single or dual source configuration. The XtaLAB Synergy-S single crystal X-ray diffractometer comes with a kappa goniometer that incorporates fast motor speeds and a unique telescopic two-theta arm to provide total flexibility for your diffraction experiment. The system is also equipped with your choice of HPC hybrid photon counting detectors, the HyPix-6000HE or the large theta coverage detectors: HyPix-Arc 100° or HyPix-Arc 150°.

In some settings, there is a desire to share instrument resources across different research groups. The XtaLAB Synergy-S in a dual-source configuration is the perfect system to be shared between protein crystallographers and chemical crystallographers: a Mo source will give the chemical crystallographers the wavelength necessary to reduce absorption from heavier elements and a Cu source, with optional continuously variable divergence slits, will give the protein crystallographer the functionality necessary to resolve large unit cells.

Benefits

- **Fast, accurate data collection** due to high-speed kappa goniometer, high-flux X-ray source, fast, low-noise X-ray detector, and highly optimized instrument control software.
- **Enhanced experimental versatility** when the dual-source option is selected from three possible wavelengths (Mo, Cu, or Ag).
- **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 with a site visit.
- **Automatically solve structures** and determine what your sample is in a few seconds before committing to a full dataset by using the "What is this?" feature.
- **Improve your ability to investigate small samples** because the solid state pixel array technology of the HyPix X-ray detectors means that X-ray photons are counted instantaneously as they arrive at the detector. There is no conversion to visible light by a scintillator so the energy of the photon can be assessed at moment of detection, leading to essentially noise free images. And noise-free images means you can count longer for weakly diffracting crystals without a loss in data quality arising from detector noise.
- **Optimize data collection speed** when you select the optional HyPix-Arc 100° or HyPix-Arc 150° curved detectors, which allow theta coverage exceeding the largest detectors while still offering the highest-performing detection technology.
- **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.

BOOK REVIEW



Review: [What If? 2: Additional Serious Scientific Answers to Absurd Hypothetical Questions](#)

By Randall Munroe
ISBN 9780525537113

What If? 2: Additional Serious Scientific Answers to Absurd Hypothetical Questions is a wonderfully entertaining continuation of *What If?* that is sure to delight anyone with a curious mind. For those familiar with Munroe's *xkcd internet comic strip*, *What If? 2?* is full of similarly hysterical cartoons.

The book is divided into 64 chapters, each answering a ridiculously silly hypothetical, ranging from "What would happen if the Solar System was filled with soup out to Jupiter?" to "What would be the most expensive way to fill a size-11 shoebox?" to "Can you use a magnifying glass and the moonlight to light a fire?" Munroe provides a detailed scientific explanation for each of these questions, complete with his trademark cartoon illustrations.

Every few chapters or so, Munroe offers an interlude of "Short Answers" (questions that have very short yes/no answers even if they seem like they don't) or "Weird and Worrying" (questions that are so borderline they bring that the more important answer really seems to be why they are being asked).

Like its predecessor, *What If? 2?* is a fun, laugh-out-loud romp, and a lovely distraction from reality. You would be remiss to miss out on it.

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 watch recordings our past sessions [here](#).

UPCOMING EVENTS:

2022 SoCal Cryo-EM Symposium, Los Angeles, CA, December 5, 2022.

Crystal 34, Society of Crystallographers in Australia and New Zealand, Bendigo, Australia, December 6-9, 2022.

CRYSTALLOGRAPHY IN THE NEWS

October 31, 2022

Researchers from Germany and Japan synthesized and characterized a series of [porous metal phosphonates](#) via hydrothermal reactions employing the linker 1,1,2,2-tetrakis(4-phosphonophenyl)ethylene and rare-earth nitrates.

November 1, 2022

Meta has developed [a language-based AI in an attempt to solve the protein folding problem](#) and deposited a preprint at bioRxiv

November 1, 2022

Researchers from the US have directly measured the [Stokes-Einstein diffusion of Cowpea mosaic virus](#) using a Rigaku XSPA-500K detector.

November 1, 2022

Researchers from the Czech Republic and Germany report on [methods to accurately determine lattice parameters from electron diffraction](#) data in part 1 of a three-part series.

USEFUL LINKS

Here are links to organizations helping Ukrainians survive the ongoing war in their homeland:

- [Help Humanitarian Efforts in Ukraine](#)
- [Donate to Children of Ukraine](#)
- [Nova Ukraine](#)
- [Razom for Ukraine](#)
- [World Central Kitchen](#)
- [Global Giving](#)
- [International Committee of the Red Cross.](#)

Here is an amazing set of pictures of an [exoplanet](#) from the James Webb Space Telescope.

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](#)

[Subscribe to Rigaku newsletters!](#)

