Volume 15, No. 5, May 2023

WELCOME

This month marks a real milestone for Rigaku and JEOL: we started the installations of XtaLAB Synergy-EDs at Institut Català d'Investigació Química (ICIQ) and The University of Warwick. These are the first installations outside Japan and outside of Rigaku. This is really quite amazing considering JEOL and Rigaku began the project in May 2020, at the height of COVID.

This month we highlight the new laboratory of Sam Yruegas at Rice University. Sam, if you are reading this, I haven't forgotten I owe you a lesson in making vacuum-sealed NMR tubes.

Our product of the month is the XtaLAB Synergy-R. We have the usual list of upcoming events, publications, video of the month, useful link and a review by Jeanette on a book that helps put the semiconductor supply chain issue in perspective.

All the best,
Joe

UPCOMING WEBINAR

The Rigaku XtaLAB Synergy-ED is a fully integrated electron diffractometer, with a seamless workflow from data collection to 3D structure determination. The XtaLAB Synergy-ED is the result of Rigaku's collaboration with JEOL, synergistically combining each partner's core technologies: Rigaku's hybrid pixel array detector (HyPix-ED) and CrysAlis^{Pro} software, and JEOL's long-standing excellence in electron beam generation and control. Using MicroED, a three-dimensional electron diffraction method, single crystals of all classes below one micron in size can be studied. The XtaLAB Synergy-ED offers the ability to determine the single crystal structure from a single grain from powder samples. In fact, one can determine the single crystal structure of multiple compounds present in a single powder sample.

There are two well-characterized polymorphs of acetaminophen with known single crystal structures. In this presentation we will explore the case of a third polymorph of acetaminophen generated in an XRD-DSC experiment with a structure determined by MicroED. This result is a major step in understanding the properties of acetaminophen and demonstrates the potential to solve many more unsolved problems in structural science.

Date/time
Wednesday, July 19, 2023 09:00 AM CDT
Register >

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy-R

The XtaLAB Synergy-R 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 before and as a side 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 detectors, HyPix-Arc 100° or HyPix-Arc 150°. For crystallographers who wish to have a powerful, well-integrated diffractometer and only need to use one port of the rotating anode, the XtaLAB Synergy-R provides the perfect combination of high-flux performance with a low-noise HPC X-ray detector.

PhotonJet-R

The PhotonJet-R comes from the same pedigree as the MicroMax-007 HF, of which there are well over 1000 units in use around the world. The PhotonJet-R X-ray source applies the lessons learned over the development and lifetime of the MicroMax™-007 rotating anode to produce a new generation, high performance rotating anode source. With the source mounted directly onto the goniometer, the XtaLAB Synergy-R provides a stable and robust solution which ensures consistently high performance. Confocal optics, designed by Rigaku Innovative Technologies, offer a high-brilliance X-ray beam and the optional continuously variable slit assembly gives the user the ability to adjust high brilliance versus low divergence depending on the needs of the sample being studied.

Proven Reliability

The PhotonJet-R source was designed with reliability in mind. Clever Rigaku engineering makes filament changes easy, like swapping a printer cartridge, with no need to realign the source each time. Scheduled maintenance involves one annual visit from a Rigaku engineer, as with all XtaLAB Synergy diffractometers, and typically takes 1-2 days. With the anode exchange program, you get the benefit of rotating anode power with the convenience of sealed tubes.

Beam Conditioning

Where overlapping peaks are a concern, e.g. large unit cells, twins or incommensurate lattices, high beam divergence is undesirable. On the PhotonJet-R source, a software controlled, motorized variable beam slit is available as an option to alter divergence to adapt the source to your sample's requirements. For those samples where intensity matters most, the slit can be fully opened giving the highest flux. For those where peak sharpness and overlap are factors, the beam can be limited to a divergence anywhere between 1 to 10 mrad.

HyPix Detectors

Rigaku's own HyPix family of HPC detectors use solid state pixel array technology to enable direct X-ray photon detection and counting. Direct X-ray photon detection 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. This leads to essentially noise free images. The HyPix detectors feature a 100 Hz frame rate which allows for data fine slicing even at the fastest goniometer speeds. The HyPix detectors incorporate dual counters enabling several modes of operation. Rapid alternating counter electronics (RACE) technology enables the 100 Hz zero dead time mode, ensures that no pixel is blind for more than a few nanoseconds during exposure to X-rays. The high dynamic range mode combines the counters to offer a massive 31-bit counter depth. Dual thresholding offers differential modes and selective signal suppression.

CrysAlis^{Pro}

The XtaLAB Synergy-R comes complete with CrysAlis^{Pro}, our user-inspired data collection and data processing software for single crystal analysis. Designed around an easy-to-use graphical user interface, CrysAlisPro can be operated under fully automatic, semi-automatic or manual control. CrysAlis^{Pro} combines automated crystal screening, the fastest and most accurate strategy software available, concurrent data reduction and automatic small molecule structure solution. CrysAlis^{Pro} can operate either in a protein or small molecule dedicated workflow. Popular third-party protein data processing packages can easily process diffraction data if desired. Visual feedback is provided for each step with clear, color-coded guidance so that both novices and experts can collect high-quality data in the shortest time possible.

AutoChem

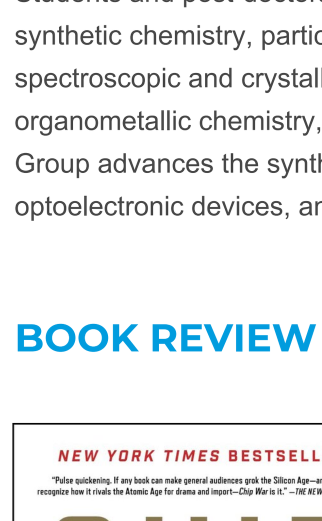
AutoChem is the ultimate productivity tool for small molecule chemists, offering fast, fully automatic structure solution and refinement during data collection. Developed in collaboration with OlexSys Ltd (Durham University, UK), AutoChem works in conjunction with Olex² where more advanced structure solution and refinement functionality exists. AutoChem is seamlessly integrated within CrysAlis^{Pro}, and forms an integral part of our 'What is this?' feature. The 'What is this?' feature gives you structures quickly and ensures you are not wasting time collecting full datasets on known samples or starting materials. It is an alternative pre-experiment option, which is used to plan your full data collections.

LAB IN THE SPOTLIGHT

Raúl Hernández Sánchez and Samantha Yruegas with Rice's new XtaLAB Synergy-S

Samantha Yruegas is the James and Deborah T. Godwin Assistant Professor of Chemistry and the Norman Hackerman-Welch Young Investigator at Rice University. Research in the Yruegas Group is focused on using earth-abundant *s*- and *p*-block metals for the development of sustainable catalysts, synthetic methodologies, and new organic materials. Students and post-doctoral researchers in the group acquire expertise in synthetic chemistry, particularly with air-sensitive manipulations, as well as spectroscopic and crystallographic techniques. With a strong emphasis on organometallic chemistry, the interdisciplinary work within the Yruegas Group advances the synthesis of innovative pharmaceuticals, optoelectronic devices, and polymers.

BOOK REVIEW



Review: *Chip War: The Fight for the World's Most Critical Technology*
By Chris Miller
ISBN 9781398504103

Chris Miller's *Chip War: The Fight for the World's Most Critical Technology* is a fascinating, deep dive into the history of the silicon microchip. Miller's narrative is engaging and moves at a fast clip, but his writing is sufficiently accessible that anyone can follow along regardless of their technological background or understanding. If anything, Miller focuses more on the international intrigue and political drama surrounding the development and manufacturing of silicon microchips over the last six decades than the actual nitty-gritty engineering of how they work.

Interestingly enough, Miller posits that the current silicon microchip shortage is not a supply chain issue, as the media and politicians have reported it, but rather a demand issue. More silicon microchips were produced worldwide in 2021 than in any other year, with a 13% increase from 2020, Miller explains. The distinction is that demand for silicon microchips was more than 13% higher in 2021 than in 2020—and the demand keeps growing faster than the supply can keep up.

As of *Chip War*'s publication in 2022, Taiwan produced 41% of all microprocessor chips and over 90% of the most advanced chips in the world. As Miller explains, "The text etched onto the back of each iPhone —'Designed by Apple in California. Assembled in China' —is highly misleading. The iPhone's most irreplaceable components are indeed designed in California and assembled in China. But they can only be made in Taiwan." This is the most important takeaway from the entire book, because underlying the currently escalating political tension between Taiwan, the United States, and the People's Republic of China is this understanding, that the technology that runs the entire world depends on silicon microchips that can only be manufactured *en masse* in Taiwan due to the country's streamlined fabricating capacities.

Indeed, while the entire book is deeply compelling, it is perhaps the final chapters that make the greatest impact. *Chip War* was published in 2022, and already, with the enormous layoffs that the tech sector has seen in the first half of this calendar year, some of the information in the latter chapters is outdated. One almost wishes Miller would publish an updated edition, although, given the rate at which global affairs intersecting with silicon microchip production are escalating, Miller—or any author for that matter—might not be able to keep up.
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 and electron diffraction, X-ray fluorescence and X-ray imaging. You can watch recordings of our past sessions here.

UPCOMING EVENTS:

PPXRD-17, Pharmaceutical Powder X-ray Diffraction Symposium, Newtown Square, PA, May 21-24, 2023.

CCCW23, 14th Canadian Chemical Crystallography Workshop, Vancouver, Canada, May 30-June 3, 2023.

NERM 2023, 2023 Northeast Regional Meeting of the American Chemical Society, Boston, MA, June 14-17, 2023.

ACA Summer Course for Chemical Crystallography, Evanston, IL, June 19-26, 2023.

ACA 2023, 73rd ACA Annual Meeting, Baltimore, MD, July 7-11, 2023.

ACS Fall 2023, San Francisco, CA, August 13-17, 2023.

IUCr 2023, 26th Congress and General Assembly of the International Union of Crystallography, Melbourne, Australia, August 22-29, 2023.

CRYSTALLOGRAPHY IN THE NEWS

April 25, 2023
Matthew Cobb and Nathaniel Cobb provide a fresh outlook on Rosalind Franklin's contribution to the solution of the structure of DNA in an editorial in *Nature*.
May 3, 2023
Scientists from Germany, Japan, Sweden and the US used XFELs to study the formation of O_2 from H_2O in crystals of photosystem II in pump-probe experiments.
May 10,2023
Researchers from US and Japan have developed a method to activate unactivated *sp*^{3} CH bonds photochemically and determined the structure of one of the products by electron diffraction.
May 10, 2023
Researchers from Singapore and China used perovskite nanocrystals to detect the angle of incidence of photons from visible light to X-rays.

USEFUL LINKS

In addition to the war in Ukraine, we have another humanitarian crisis in Sudan. It seems that medical aid is the most critical need now. Doctors without Borders is a reputable organization and is providing aid in Sudan.

Here is a link that provides useful information regarding relief efforts for Ukraine: Here's how you can help the people of Ukraine: NPR

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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