



Volume 14, No. 7, July 2022

WELCOME

The US recently celebrated the Fourth of July. At dawn on July 2nd, I took down the Ukraine flag from the flagpole at my house and raised the American flag until sunset on July 4th. The next morning, I raised the Ukraine flag again as a reminder that this war is still ongoing and should not be forgotten. The first set of useful links again point to organizations that are providing support to Ukraine. I wanted to highlight something positive (and not COVID positivity rates): the first images from the James Webb Space Telescope. The images are simply amazing and awe-inspiring. They should give us pause to think about where we are in the cosmos.

This month we highlight the recent installation of a XtaLAB Synergy-S at the University of Southern California. Our product of the month is the XtaLAB Synergy-DW VHF, which has made an impact on social media. We have a few interesting articles from the last month and a second set of useful links pointing to CCP4-ED. Finally, Jeanette has some summer reading suggestions.

Stay positive, test negative,
Joe

RESEARCHERS IN THE SPOTLIGHT

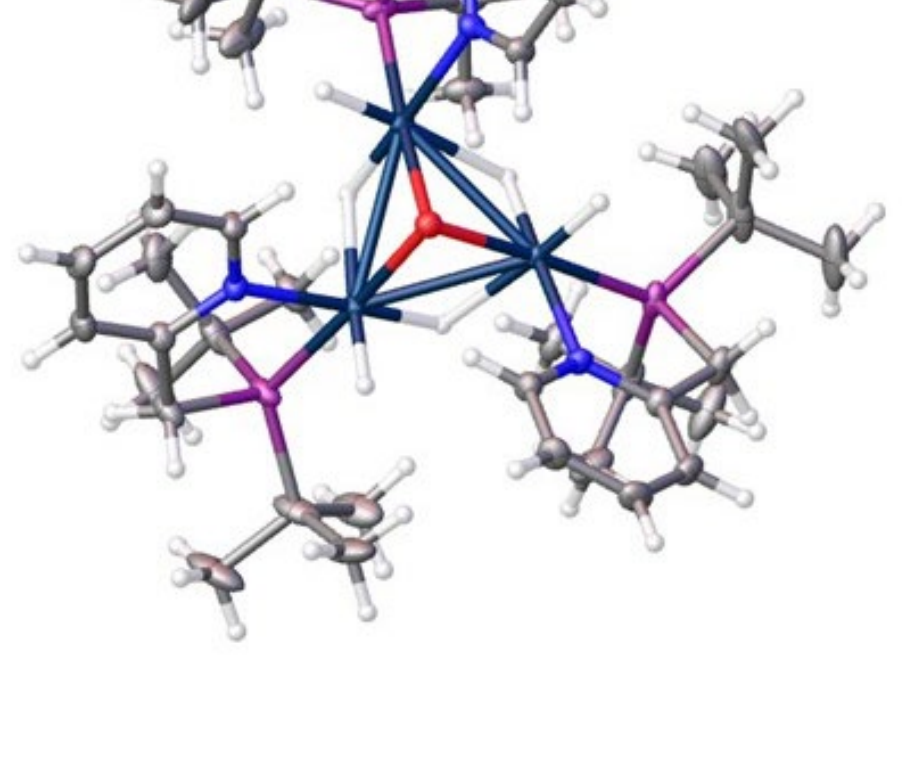
The University of Southern California, Department of Chemistry recently commissioned their XtaLAB Synergy-S. The diffractometer is shared by Professors Travis Williams and Mark Thompson.



Travis Williams and Mark Thompson of the University of Southern California, Department of Chemistry with their dual XtaLAB Synergy-S

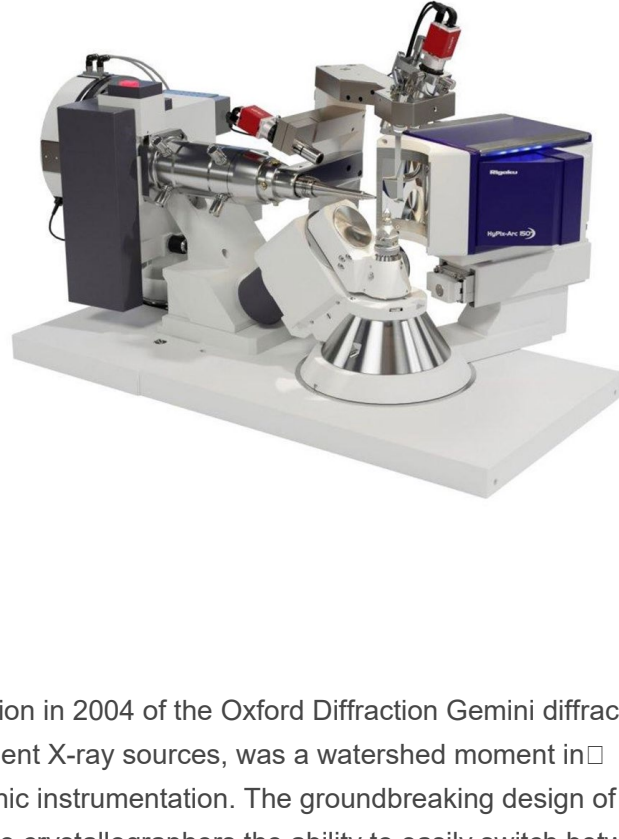
Mark Thompson's research is in the area of molecular materials for organic electronic applications. He works extensively with metal complexes, which find applications as emitters in organic LEDs (both displays and solid-state lighting), light absorbers and carrier transporters in solar cells and as sensitizers for producing solar fuels. He has a group of about 15 students and postdocs that use X-ray crystallography as a key step in understanding the properties of each new material.

The Williams lab studies catalysis, approaching problems ranging from hydrogen on demand to alkaloid total synthesis. They use crystallography to show how simple transition metal pre-catalysts can convert to multi-metallic active species in complex catalytic systems. Below is an example of a triridium $\text{Y}_3\text{-oxo}$ compound that they characterized on their new XtaLAB Synergy-S system in a dehydrogenation catalysis project. Structure courtesy of Van Do and Nick Alfonso.



PRODUCT IN THE SPOTLIGHT

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 evolution 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. It is the perfect diffractometer for a core facility where protein crystallography and small molecule crystallography are both practiced.

Configuration

The XtaLAB Synergy-DW VHF diffractometer contains a PhotonJet-R X-ray source that is based on the proven, low-maintenance MicroMax-007 HF microfocus rotating anode X-ray generator. The target is constructed with two different X-ray source materials (the following combinations are available: Mo/Cu, Cu/Cr, Cu/Co, Cu/Ag, and Ag/Mo; only Mo and Cu optics are available with VHF style optics) and is coupled with an auto-switching dual-wavelength optic. Two wavelengths of X-ray radiation are available at the click of a button and switching between wavelengths takes only 5 minutes. Rounding out the XtaLAB Synergy-DW VHF configuration is the fast and efficient four-circle kappa goniometer which is coupled with Rigaku's Hybrid Photon Counting (HPC) X-ray detector, the HyPix-6000HE (or optionally the curved, large theta coverage detectors, HyPix-Arc 100° or HyPix-Arc 150°) which has essentially no readout noise, no dark noise and high dynamic range. All of this controlled by the CrysAlis^{Pro} diffraction software package, with sophisticated algorithms to tie the hardware together to minimize the time it takes to measure and solve single crystal X-ray structures.

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, proteins, twinned or incommensurate lattices, high beam divergence is undesirable. On PhotonJet sources, 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.

CrysAlis^{Pro} v42

The XtaLAB Synergy-DW VHF 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, CrysAlis^{Pro} 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 messages so that both novices and experts can collect high-quality data in the shortest time possible.

AutoChem

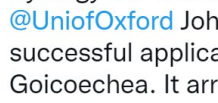
AutoChem is the ultimate productivity tool for small molecule chemists, offering fast, fully automatic structure solution and refinement during data collection. Developed in collaboration with OlexSys Ltd (Durham University, UK), AutoChem works in conjunction with Olex2 where more advanced structure 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.

Comments from the TwitterVerse about the XtaLAB Synergy-DW



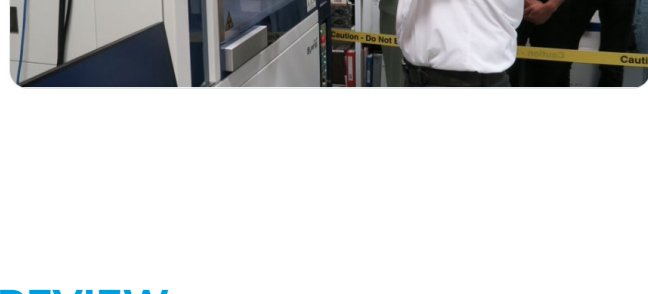
A.J. Fitzpatrick
@AJFitz_Chem

This machine has blown my mind. #crystallography #NTUChemistry

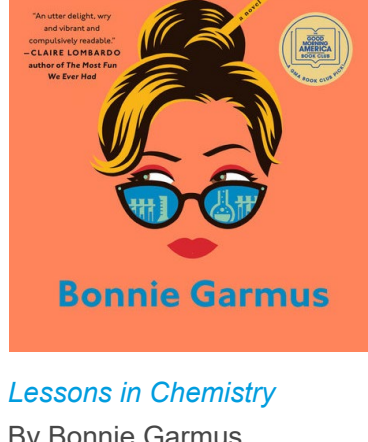


Oxford Chemistry
@OxfordChemistry

"First light" for Department's new X-ray Rigaku Synergy DW diffractometer, purchased with @EPSRC & @UniofOxford John Fell Fund funding following a successful application by Richard Cooper & José Goicoechea. It arrival means we are able to collect data on smaller crystals & faster



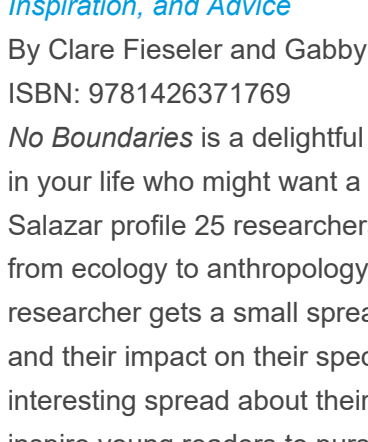
BOOK REVIEW



Lessons in Chemistry
By Bonnie Garmus
ISBN: 9780385547345

Lessons in Chemistry is a compelling, albeit fictional, portrait of a female research chemist in Southern California in the 1950s and 60s who, as luck—or rather, lack of luck—would have it, finds herself a single mother supporting a young daughter and hosting an evening cooking show called *Supper at Six*. Elizabeth Zott becomes a national sensation with her chemistry-first approach to the culinary arts, brewing coffee with Bunsen burners and always ending her show with a simple tagline that was ahead of her time: "Children, set the table. Your mother needs a moment to herself."

Any more information would spoil this incredible story, which is frustratingly relatable—think sexism in the workplace—and at times devastatingly heartbreaking. It seems inappropriate to describe Zott's story—although it is a work of fiction—as entertaining. But *Lessons in Chemistry* is one of the best fiction books of 2022. You won't be able to put it down. It's perhaps a bit too heavy for a beach read, but worth cracking open this summer nonetheless.



No Boundaries: 25 Women Explorers and Scientists Share Adventures, Inspiration, and Advice
By Clare Fieseler and Gabby Salazar
ISBN: 9781426371769

No Boundaries is a delightful read for any young women (or young men) in your life who might want a fun read for summer vacation. Fieseler and Salazar profile 25 researchers across various fields of scientific research, from ecology to anthropology to planetary science to volcanology. Each researcher gets a small spread detailing their background, their research, and their impact on their specialty, which is followed by a fun and interesting spread about their respective field of research designed to inspire young readers to pursue their own avenues of research and experimentation (safely) at home.

Reviews by 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.

VISIT US AT:

- ACA Annual Meeting , Portland, OR, July 29-August 3.
- 33rd European Crystallographic Meeting, Versailles, France, August 23-27.
- 44th International Conference on Coordination Chemistry, Rimini, Italy, August 28-September 2.
- 8th International Conference on Metal-Organic Frameworks and Open Framework Compounds, Dresden, Germany, September 4-7.
- The Pittsburgh Diffraction Conference, Lemont, IL, October 2-4.
- 73rd Southeastern Regional ACS Meeting (SERMACS 2022), San Juan, Puerto Rico, October 19-22.

CRYSTALLOGRAPHY IN THE NEWS

May 24, 2022: Researchers from the UK and US have synthesized neptunium compounds with dative single and multiple Np-C bonds.

June 15, 2022: Scientists from China have synthesized and structurally characterized a monolayer fullerene network.

June 23, 2022: Researchers from Leibniz-Institut für Katalyse have synthesized and characterized a versatile Ni(II) catalyst for hydrogenating nitriles to amines.

June 28, 2022: Researchers from Japan have synthesized and characterized a set of perfluoro[n] cycloparaphenylenes where n=10, 12, 14 and 16.

June 30, 2022: Researchers from the Scripps Research report the synthesis of GB18 the main psychotropic chemical from *Galbulimima* bark, as well surveying potential targets for GB18.

July 1, 2022: Researchers from Stockholm University report propose strategies for obtaining accurate structure models with interpretable ADPs based on kinematical refinement against single crystal electron diffraction data.

USEFUL LINKS

Here 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 a great poster on simulating dynamical diffraction using multislice and Bloch wave approximations [pdf] from the CCP4-ED web page. There is also a great silent video that takes you through the Bloch wave approximation [mp4], starting with diffraction basics, in less than 3.5 minutes.

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

