

Volume 15, No. 12, December 2023

## INTRODUCTION

Another great article for crystallographers came out this month, this one by a team led by Tom Terwilliger. The article demonstrates that, while AI-generated can be useful, the ground truth for protein structure is provided by experimental methods; that is, density from crystallographic studies.

This month, Fraser interviews J. Derek Woollins, formerly of Khalifa University and, before that, the University of St. Andrews. As I have done in the past, we highlight one of our own labs for the December issue—this time the newly renovated labs at Rigaku Europe SE (RESE) in Frankfurt. We have chosen Intelligent Optic Module, a fully automated optical alignment system we introduced at IUCr, for the product of the month.

Jeanette is getting married in January, so I gave her the month off. We'll have a review from her in January. Instead, I review a privately published book *Memoir of the Years in Exile (1939-1946)* by Paulina Wlodawer.

It is the holiday season, so I will remind everyone of the words from "The Secret of Christmas" by Van Heusen and Cahn: "It's not the things you do at Christmas time, it's the Christmas things you do all year through." Think about this sentiment. If we all try a little harder, the world will be a better place.

With that thought in mind, Happy Holidays and a Prosperous New Year.

Be safe,  
Joe Ferrara

## 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 WEBINAR: TOPIQ | Pump-multiprobe

**Photocrystallography on the XtaLAB Synergy-R system**  
Wednesday, January 31, 2024 at 09:00 CST

**Presenter: Dr. Lauren Hatcher, Cardiff University**

In this Webinar we will describe a new setup, developed in collaboration between Cardiff University and Rigaku, that enables the collection of pump-probe Photocrystallography data down to a time-resolution of 10 ns, producing full, 3D structures at regular time-points to create 3D molecular movies.  
[Register now](#)

### UPCOMING EVENTS: CCP4 Study Weekend 2024

Decision making in MX - how to be a productive structural biologist, EMCC, Nottingham, UK & Virtual, January 3-5, 2024.

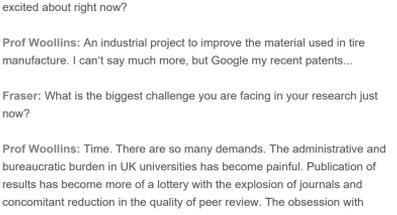
### Rigaku School for Practical Crystallography

January 15-19 and 22-26, 2024.

### 2024 ACADEMY OF CHEMICAL Crystallography at Purdue University

from June 23-30, 2024.

## TOPIQ | Pump-multiprobe Photocrystallography on the XtaLAB Synergy-R system



In this Webinar we will describe a new setup, developed in collaboration between Cardiff University and Rigaku, that enables the collection of pump-probe Photocrystallography data down to a time-resolution of 10 ns, producing full, 3D structures at regular time-points to create 3D molecular movies.

[Read more about TOPIQ | Pump-multiprobe Photocrystallography on the XtaLAB Synergy-R system >](#)

Wednesday, January 31, 2024 at 09:00 CST  
[Time Zone Converter](#)

Presenter  
Dr. Lauren Hatcher, Cardiff University

**REGISTER NOW**

## INTERVIEW WITH A RESEARCHER



Professor J. Derek Woollins

J. Derek Woollins, FRSC FRSE is a chemist who was most recently Provost of Khalifa University, Abu Dhabi. Prior to that, he was Vice Principal of Research and Innovation and Provost of St Leonard's College at the University of St Andrews. He is a Fellow of the Royal Society of Chemistry since 1994[5] and a Fellow of the Royal Society of Edinburgh.

Fraser: How would you describe your primary research interest to a non-specialist in one or two sentences?

Prof Woollins: I am interested in making new molecules and materials with useful properties. The key driver is to develop synthetic chemistry but with a view to useful outcomes, such as lower energy use in industrial processes and molecules with unusual properties.

Fraser: What research project(s) are you working on that you are most excited about right now?

Prof Woollins: An industrial project to improve the material used in tire manufacture. I can't say much more, but Google my recent patents...

Fraser: What is the biggest challenge you are facing in your research just now?

Prof Woollins: Time. There are so many demands. The administrative and bureaucratic burden in UK universities has become painful. Publication of results has become more of a lottery with the explosion of journals and concomitant reduction in the quality of peer review. The obsession with citation metrics and things like "h-indices" is damaging the quality of academic research.

Fraser: Looking forward, where do you see the future of crystallography in the home lab leading?

Prof Woollins: In my lifetime, home lab crystallography has become much more accessible to average synthetic chemists like me. It has a much stronger analytical/characterisation flavour nowadays.

Automation of processing and structure solution—particularly for twinned/multiple crystals—could be improved further and better integration of databases with new results to enable assessment of the structures would be great. The recent developments in electron diffraction are impressive.

Fraser: Looking back, how has crystallography in the home lab changed for you since the start of your career?

Prof Woollins: Yes, both hardware and software have improved. Area detectors changed things greatly, with image processing becoming a major part of the process, but enabling smaller and more difficult samples to be studied and very quick data collections on traditional size crystals.

Fraser: Anything else you'd like to share with our readers?

Prof Woollins: Since I work on non-NMR active systems, crystallography has been essential for progress. Whilst amateurs like me can collect and solve routine data, there is still a place for real experts when there is a challenging problem. When you do have a really difficult sample and the crystallographer gets an answer, it may not look great in checkCIF. Do consider if the outcome is fit for purpose, i.e., the connectivity may be enough to enable you to move on with the project...checkCIF is a useful but blunt instrument!

## LAB IN THE SPOTLIGHT

The Single Crystal Application Lab at Rigaku Europe SE, strategically located near Frankfurt airport, stands as a pinnacle of cutting-edge research facilities. Our lab is equipped with state-of-the-art X-ray and electron diffraction instruments, showcasing a commitment to advancing scientific exploration. Our instruments include:

- XtaLAB Synergy-S: This instrument features dual-source microfocus sealed tubes (Ag, Mo, or Cu) and a HyPix ARC100 detector.
- XtaLAB Synergy-DW: With a dual-wavelength rotating anode source (Mo and Cu), the FLOW robot for high throughput workflows, and a HyPix-Arc 150° detector.
- XtaLAB Synergy-ED: Tailored for electron diffraction, this instrument is equipped with provisions for cryo transfer and high-temperature holders.

Our dedicated scientific team comprises six experts with diverse experience in single crystal and micro-powder diffraction, along with expertise in related total scattering methods. They excel in applications such as the analysis of MOFs, organometallic compounds, organic materials, macromolecular structures, charge density analysis, absolute structure determination, and more.

Collaboratively, we offer comprehensive services encompassing application training, both in-person and remote demonstrations, unparalleled customer support, and a specialized electron diffraction structure solution service tailored to industry needs.

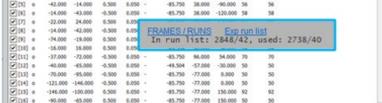
If you're interested in experiencing our cutting-edge instrumentation firsthand, we welcome you to get in touch to arrange a visit to our lab. Email us at [info@rigaku.com](mailto:info@rigaku.com) to make an appointment.



## PRODUCT IN THE SPOTLIGHT

### Intelligent Optic Module (IOM) - A FULLY AUTOMATIC OPTIC ALIGNMENT SYSTEM

Achieve peak source performance any time with IOM automated alignment



#### Effortless Intensity

Automatic beam alignment for consistent performance, the XtaLAB Synergy-DW VHF can now be equipped with our new Intelligent Optic Module (IOM) for fully motorized automatic beam alignment. With encoders on every axis, IOM puts the beam exactly where you need it with high reproducibility, perfect for the smaller samples commonly studied today. IOM also lets you achieve maximum intensity from your source by automatically maximizing the intensity so you can achieve peak performance at all times.

#### Peak Performance

With automatic alignment, your source can maintain peak performance all the time. Perfect alignment can be achieved within a few minutes to keep your system ready for the smallest and most challenging samples.

#### Precision Engineering

Reproducibility  
The IOM device has been designed with encoders on each motor to ensure it knows its exact position. When aligning the beam, this enables the best position to be automatically found and remembered so optimal alignment can be easily recovered.

Safety  
Manual alignment of the X-ray sources often requires direct access to tubes and screws inside the radiation safety enclosure. This represents a risk of exposure to X-ray radiation and thus is often left to service engineers to perform. The IOM device allows fully remote alignment of the X-ray optic while the X-ray safety enclosure is safely interlocked.

Simplicity  
X-ray source alignment has never been easier with the IOM device attached to your source. The X-ray optic can be aligned either using manual point and click to point the beam at the sample or automatic alignment for maximum intensity in just a few minutes.

More independence  
The IOM gives unprecedented control over the optic position, all controlled via a software interface. This means that service engineers no longer need to be present on-site to accomplish full optic alignment. Either use our automatic routine or adjust the alignment yourself with an easy-to-use, intuitive software interface. Still not confident? Our service engineers can step in and perform alignment and source diagnostics over the internet, minimizing your service costs.

#### Unique Benefits of IOM

- Fully automatic optic alignment for reproducible, safe and simple alignment
- Peak performance at all times
- Remote source optimization from the next room or the next continent
- Align your source with the safety enclosure closed and interlocked.

[Learn more >](#)

## ACA SUMMER COURSE 2024

It is with great pleasure that the organizers of the ACA Summer Course announce the 2024 ACA Summer Course in Chemical Crystallography. The course will be held at Purdue University from June 23-30, 2024. For more details, please check the web page at <https://acasummercourse.net/>

Applications for the course will open on January 1, 2024.

For international attendees requiring a visa to enter the United States: There have been increasingly long processing periods in recent years to obtain a B1 visa. If you are planning to apply for the course, please contact us as soon as possible.

Should you have any questions, please email [info@acasummercourse.net](mailto:info@acasummercourse.net)

### The Organizers

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## TIP OF THE MONTH

### Tip of the Month: Run & Frame Selector Tool

By Chris Schürman

At times, something goes south during data collection and unwanted effects need to be treated during data processing. The crystal can jump, drop or completely lose its diffraction power; the crystal might get in the way and block the beam; the cryo can fail or create ice on the crystal. For any of these cases, the affected frames should be excluded from the integration or the frames need to be integrated in batches with later merging of the data in case of strongly jumping crystals. For the task of (de-)selecting runs and frames for integration, the run- and frame selector tools were designed and integrated in CrysAlisPro in Version 41 (2020).



Figure 1. Data Reduction Tab.

The tools can be found in the **Data Reduction** tab. When you click on the experiment name, the program toggles between the full Exp(eriment) run list and the custom **FRAMES/RUNS** list. When you select **FRAMES/RUNS**, the corresponding **Select Runs** and **Frame Selector** tools can be opened. (As a side note, the **Repair Dataset** option will check the frames folder for existing frames and rebuild the run list accordingly.)

The **Select Runs** window presents a table of all existing runs with the option to (un-)select them by the click of a checkbox. Using Ctrl or Shift, multiple runs can be selected at once. The updated number of frames will be displayed in the **Data Reduction** tab.



Figure 2. The Select Runs Window.

Likewise, the **Frame Selector** tool can be opened. This dialog allows you to change frames selection status, change display settings and use frames auto selector functions. To toggle the individual frame selection status you either need to click the checkbox "Used" or press **F2**. Frame selection by pressing the corresponding buttons or the F3-F8 shortcuts, the frame status can be toggled for the following set of frames:

- **F3**: from first frame in current run till the current frame
- **F4**: from current frame till the last frame in current run
- **F7**: sets all frames in the experiment to used
- **F8**: sets all frames in the experiment to not used



Figure 3. Auto selector options.

A special feature in the **Frame Selector** is the **Auto selector option**. For each frame, a general signal intensity can be calculated. By selecting the corresponding checkbox, this is displayed in the **Frame Selector** status bar. This signal can be used in the **Auto selector options** dialog to filter out empty frames with a particularly low intensity or alternatively all frames in a given series with a sufficiently high threshold.

Final remarks: When any frame status is changed for the first time, in the background a **FramesSelectionStatus.ini** file is created, which logs the selection status of all frames and can be deleted using the "Delete status file" button. When using "Beamstop/Let shadow overlay", "unused frames are displayed with an inverted coloring scheme and when integrating the data with the **Data Reduction Assistant**, the selected/skipped frames are displayed and the **Run Selector** dialogue is linked via the **Multi Selection Button**.



Figure 4. Data Reduction Assistant.

## BOOK REVIEW



**Memoir of the years of exile (1939-1946)**  
By Paulina Wlodawer

Review: [Memoir of the Years of Exile \(1939-1946\)](#)

By Paulina Wlodawer

You may recognize the surname of the author, who is, in fact, the mother of Alex Wlodawer of the National Cancer Institute. I saw Alex at the IUCr and we were discussing our Jewish heritage and family histories. Alex mentioned his mother had written a memoir of her life during World War II and I asked for a copy. The memoir was written in Polish forty years after WWII by Paulina. Google was used to translate from the original Polish and corrected by Alex. Anna Pyżewska provided the copious footnotes.

The book follows Paulina, her husband, and her father from Krakow to the western USSR following the invasion of Poland by the Third Reich. From there, they were deported to Asino in western Siberia, where Paulina became a nurse at a work camp. In 1942, when Hitler invaded the USSR, Paulina and her family were relocated to Tashkent in Uzbekistan, where they spent the rest of the war until repatriated to Poland in 1946.

The details of daily life are so vivid that it is hard to believe it was written 40 years after the fact. For example, I found myself smelling the pine in the housing in Asino. The chapters dealing with the later years are more compressed in time, I suspect much like COVID is a blur to many of us.

At this time, publication of the memoir (in Polish only) is still being decided. However, if you would like to read the English version, as I have, you can obtain a copy by sending an e-mail to Alexander Wlodawer ([wlodawer@aci.com](mailto:wlodawer@aci.com)).

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