

INTRODUCTION

Another great article for crystallographers came out this month, this one by a team led by Tom Terwilliger. The article demonstrates that, while Al-

place.

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 iOptix, 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 titled Memoir of the Years in Exile (1939-1946) by Paulina Włodawer. 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

With that thought in mind, Happy Holidays and a Prosperous New Year. Be safe, Joe Ferrara

Joy to the

World! All of us at Rigaku wish you

and your family

joyous holidays and

a happy new year

Dr. Lauren Hatcher

Q Rigaku **TOPIQ | Pump-multiprobe**

Photocrystallography on the XtaLAB

Synergy-R system **@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 ms, producing full, 3D structures at regular time-points to create 3D molecular

A RIGAKU WEBINAR

Dr. Lauren Hatcher, Cardiff University

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

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INTERVIEW WITH A RESEARCHER

Professor J. Derek Woollins J. Derek Woollins, FRSC FRSE is a chemist who was most recently Provost

and molecules with unusual properties

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

excited about right now?

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.

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 sized crystals.

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!

The Single Crystal Application Lab at Rigaku Europe SE, strategically

facilities. Our lab is equipped with state-of-the-art X-ray and electron diffraction instruments, showcasing a commitment to advancing scientific

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LAB IN THE SPOTLIGHT

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more.

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Automatic beam alignment for consistent performance, the XtaLAB Synergy-DW

automatic beam alignment. With encoders on every axis, iOptiX puts the beam exactly where you need it with high reproducibility, perfect for the smaller samples commonly studied today. iOptiX also lets you achieve maximum intensity from

VHF can now be equipped with our new iOptiX device for fully motorized

The iOptiX 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 Safety Manual alignment of X-ray sources often requires direct access to knobs 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 iOptiX device allows fully remote alignment of the X-ray optic while the X-ray safety

X-ray source alignment has never been easier with the iOptiX 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

The iOptiX 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

The Organizers

TIP OF THE MONTH

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

list and the custom FRAMES/RUNS list. When you select

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

FRAMES/RUNS, the corresponding Select Runs and Frame Selector tools

 F8: sets all frames in the experiment to not used F2 - toggle status of current frame F3 - toggle status (based on current frame) of all frames in range: from first frame in current run till current frame F4 - toggle status (based on current frame) of all frames in range: from current frame till last frame in current run F7 - set status of all frames in experiment to used Auto selector options (1.0.1) Start F8 - set status of all frames in experiment to not used Frame: 10 Status file OK Run: 3 Display settings Show all frames (2738) Frame: 40 Run: 3 C Show only used frames (2737) C Show only not used frames (1) Threshold: 99999 Status: not used (F2 to toggle) Run: 3 correlation

-85.75 -40.00 -14.00 38.00 0.05 0.05 -42.00 0.50 -85.75 -14.00 38.00 -43.00 -14.00 0.50 -85.75 0.05 -22.00 24.00 0.50 -49.50 19.00 -14.00 -85.75 -42.00 0.50 38.00 0.05 0.05 -74.00 -19.00 0.50 -49.50 96.00 0.50 -16.00 16.00 -49.50 96.00 0.05 --72.00 -37.00 0.50 -85.75 96.00 By default the whole experiment will Edit start num of selected run evaluated. To modify this behaviour edit the run list Edit end num of selected run

Button.

(1939 - 1946)Paulina Włodawer

of Alex Włodawer 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

since 1994[5] and a Fellow of the Royal Society of Edinburgh. Fraser: How would you describe your primary research interest to a nonspecialist 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

Fraser: What research project(s) are you working on that you are most

of Khalifa University, Abu Dhabi. Prior to that, he was Vice Principal of

University of St Andrews. He is a Fellow of the Royal Society of Chemistry

Research and Innovation and Provost of St Leonard's College at the

Fraser: Looking back, how has crystallography in the home lab changed for you since the start of your career? **Fraser:** Anything else you'd like to share with our readers?

(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.

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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 iOptiX** Fully automatic optic alignment for reproducible, safe and simple

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

#run type start end width time omega detector kappa phi # frames # done -43.000 -17.000 0.500 0.050 --85.750 38.000 -60.000 52 52 -14.000 -43.000 -0.500 0.050 --85.750 38.000 -30.000 58 -57.000 -28.000 0.500 0.050 --85.750 57,000 -40,000 -14,000 0.500 0.050 --85.750 38,000 0.000 52 -42,000 -14,000 0.500 0.050 --85.750 38,000 -90.000 -43.000 -0.500 -22,000 24,000 0.500

0.05

0.050 +

0.050 -

0.050 -

0.050

0.05 0.500

-0.500

-0.500

-0.500

0.500

displayed in the Data Reduction tab.

-14.000 -42.000 -0.500

-19.000

16.000

-72,000

-65,000

-74.000

-16.000

-37,000

40,000

-121.000 -146.000

-146.000 -100.000

₹[8] o

₹[11] o

√ [12] o

₹[13] o **₹**[14] 0

₹ [15] o

[9]

Signal: 197 Change status of frames automatically Frames in current run FRAMES/RUNS Exprunist
Run: 2848/42, used: 2738/40(skip:31)

> *.rodhypix ▾ width exposure omega detector kappa end ^ 0.50 0.05 -60.00 0, 0 0.50 0.05 -85.75 -30.00 0 38.00 0.05 0.05 0.50 -85.75 57.00 0.00 58 0.50 0.00 52 -90.00 56 38.00 -120.00 58 120.00 92 120.00 56 54.00 110 1, 54.00 64 54.00 70 Multi selection Figure 4. Data Reduction Assistant.

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

Figure 3. Auto selector options.

completely lose its diffraction power; the crystal mount can 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 Data Reduction FRAMES/RUNS ed: 2848/42 In run list: 2848/42, Exp run list 2848/42, used: 2848/42 RUNS RUNS Exp run list ist: 2848/42, used: 2848/42 Select runs Frames selector ANALYSIS Repair dataset lone: 2848 Reflections tested: 7428. used: 6142 Figure 1. Data Reduction Tab.

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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

Allen Oliver (University of Notre Dame), aoliver2@nd.edu Matthias Zeller (Purdue University), zeller4@purdue.edu

Charlotte Stern (Northwestern), c-stern@northwestern.edu

Christos Malliakas (Northwestern), c-malliakas@northwestern.edu

Nathaniel Barker (Northwestern), nathaniel.barker@northwestern.edu

case of strongly jumping crystals. For the task of (de-) selecting runs and frames for integration, the run- and frame selector tools have been integrated in CrysAlisPro in Version 41 (2020).

-77.000 0.050 -₹ [16] o -90.000 -65.000 -85.750 150.000 ₹[17] o -103.000 -71.000 0.050 --49.504 -57.000 -30.000 ₹[18] o -153,000 -81,000 0.500 0.050 --85.750 -38,000 -180,000 -145.000 -117.000 [√ [19] o 0.500 0.050 --85.750 -96,000 -54.000 -109.000 0.050 --49.504 -125,000 0.000 ₹ [20] o -83.000 30,000 -112.000 0.050 --49.504 √ [21]
o -78.000 -0.500-125.000 √ [22]
o 37.000 64,000 0.500 0.050 -106.182 -57.000 -120.000 54 ₹[23] o 105.000 -77.000 80.000 -0.500 0.050 -106.182 -30.000 0.050 -[25] 0 34,000 66,000 0.500 0.050 -106.182 -57,000 -30.000 ₹ [26] o 60,000 35,000 -0.5000.050 + 106.182 -57,000 0.000 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. Accordingly: by

-85,750 96,000

-85.750

-85.750

-57,000

-77.000

-77.000

FRAMES/RUNS Exprunlist
In run list: 2848/42, used: 2738/40

54,000

0.000

150.000

92

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/Jet 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 Proffit: CrysAlisPro data reduction assistant (1.2.0) CRYSALIS Profile fitting data reduction Step 2: Experiment run list for data reduction

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 tab. 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.

Run list: C:\Users\christian.schuermann\OneDrive - Rigaku Americas Skip (Frames selector): 31 Image dir: C:\Users\christian.schuermann\OneDrive - Rigaku Americas end start -43.00 -14.00 -43.00 -57.00 -28.00

BOOK REVIEW Memoir of the years of exile

Review: Memoir of the Years of Exile (1939-1946) By Paulina Włodawer You may recognize the surname of the author, who is, in fact, the mother

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.

obtain a copy by sending an e-mail to Alexander Włodawer

(wlodawer@aol.com).

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

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30, 2024.

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2024 ACA Summer Course in Chemical Crystallography at Purdue University from June 23-

We now have a full-scale war in

the Middle East, earthquakes In Afghanistan an ongoing war in

Ukraine, and humanitarian crises elsewhere. With some much

organizations like the International

Movement, so they can distribute

suffering, perhaps it is a good time to donate to larger relief

Red Cross and Red Crescent

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CrysAlis^{Pro} software for single

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crystal data processing.

techniques in their own

hope that you will share information about your own

information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other

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Twitter feed.

how to be a productive structural biologist, EMCC, Nottingham, UK

CCP4 Study Weekend

UPCOMING WEBINAR: TOPIQ | Pump-multiprobe XtaLAB Synergy-R system 09:00 CST

watch recordings of our past sessions here.

Photocrystallography on the Wednesday, January 31, 2024 at 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 pumpprobe Photocrystallography data

at regular time-points to create 3D

X-ray imaging. You can

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

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