



Volume 15, No. 2, February 2023

WELCOME

When you receive this newsletter, you will have about one more week to register for the TOPIQ Webinar: XtaLAB Synergy-ED Progress and Latest Results, which will be presented by Robert Bücker on February 23. If you haven't registered already, I strongly encourage you to do so if you are interested in electron diffraction for single crystals.

In recognition of Black History Month, we highlight Howard University, which was federally chartered in 1867 and today provides 120 different degree programs, the most of any historically black college or university in the US. It is the site of one of the most recent XtaLAB Synergy-S installations.

This month we have an old/new product in the spotlight, ACTOR 2. We have updated the robot arm to a modern Universal Robotics arm while maintaining the same functionality the venerable ACTOR system provided, even keeping the same API.

We have the usual list of interesting papers, useful links concerning humanitarian aid for Turkey and Syria, and a cool video. Finally, Jeanette reviews *Breathless: The Scientific Race to Defeat a Deadly Virus.*

I'd like to remind you that the IUCr abstract deadline is Tuesday, February 21, in case you are planning to submit something. I look forward to seeing you there and to an exciting Congress.

Be safe, Joe

LAB TOUR AT THE DGK



Please join us for a tour of Rigaku's laboratory in Neu-Isenburg during DGK this March. The tour will be on Thursday March 30th from 2-6 pm, and we will provide transport to and from the DGK venue if needed. If you'd like to attend, please register at this link. Places are limited so be sure to register early if you'd like to attend.

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 WEBINAR

TOPIQ Webinar: XtaLAB Synergy-ED Progress and Latest Results, February 23, 2023.

UPCOMING EVENTS:

Pittcon 2023, Philadelphia, PA, March 18-22, 2023

ACS Spring 2023, Indianapolis, IN & Hybrid, March 26-30, 2023

DGK 2023, Frankfurt, Germany, March 27-30, 2023

BCA Spring Meeting 2023, Sheffield. UK, April 3-6, 2023

The ACA Summer Course will be held at Northwestern University from June 19-26, 2023, and is organized by Matthias Zeller (Purdue University), Christos Malliakas (Northwestern University), Charlotte Stern (Northwestern University) and Allen Oliver (University of Notre Dame). Applications can be found at the Course website.

CRYSTALLOGRAPHY IN THE NEWS

January 11, 2023

Researchers from the US have synthesized and characterized a series of MOFs that can absorb

PRODUCT IN THE SPOTLIGHT

ACTOR 2: AUTOMATED CRYSTAL TRANSPORT ORIENTATION AND RETRIEVAL ROBOT

Automatic sample mounting, single crystal X-ray screening and data collection

Features

- Completely automated sample mounting, centering and data collection
- Integrated sample ranking and data collection strategy algorithms.
- Choice of dewar base plates for use with either ACTOR, ALS, Uni-Puck sample holders. (Tools and magazines for ALS and Uni-Puck must be purchased separately.)
- Storage capacity: up to 112 samples per dewar, up to 3 dewars depending on puck system in use.



The ACTOR[™] system is a proven commercial solution for automating routine crystal screening and data collection at both synchrotron beam lines and home laboratories. Compatible with almost any goniometer and detector combination, the ACTOR 2 builds on the successful ACTOR with a new robotic arm, the Universal Robotics UR5e. The ACTOR system provides a reliable, consistent way to mount samples while at low temperature, and ensures anyone can safely transfer sensitive samples to the goniometer and back. The 4th generation gripper minimizes formation of ice and mimics mounting by hand with cryo tongs such that the sample is immediately bathed in the cold stream of the cryo device when mounted. A robotic sample changer also enables unattended operation for extended periods of time day and night, thus maximizing return on investment.

Rapid automatic crystal screening

ACTOR 2 allows you to screen up to 30 samples per hour. Adding automation to your structure solution pipeline also complements the high throughput needed for fragment-based screening projects and structural genomics programs. ACTOR 2 enables you to quickly screen many crystals for optimal diffraction qualities and cryo-conditions and includes ranking software to assist you in comparing samples and finding the best crystals for data collection.

Shorten the crystallization to structure pipeline

ACTOR 2 allows you to effectively shorten the time gap between crystallization and structure solution. ACTOR was the first commercial automated crystal mounting robot and won the 2002 R&D 100 Award for up to 30% their own weight in ammonia.

January 19, 2023

Scientists from China, Spain, Sweden and the US used electron diffraction to characterize a zeolite with extra-large pores through a 1D to 3D topotactic condensation.

January 27, 2023

Scientists from Australia, Germany, Italy and the UK synthesized and characterized a periodic assembly of identical zinc-containing clusters connected uniformly in a welldefined but disordered fashion to give a topologically aperiodic microporous network creating a Truchet tiling.

February 2, 2023

Scientists from Osaka University developed a method to add a single carbon to atom α , β unsaturated amides from Nheterocyclic carbenes and used crystallography to verify the result for one compound.

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.

As the war in Ukraine continues, we have another humanitarian crisis in Turkey and Syria. USA Today has provided some information as to where one can support relief effort in those countries.

VIDEO OF THE MONTH

Here is a cool video of a liquid metal robot escaping jail. A T-1000, it's not. Watch This Liquid Metal Robot Escape from Jail, Just Like *Terminator 2*.

technical innovation. Today over 70 ACTOR robots are in operation in home labs and at beamlines around the world. ACTOR 2 can increase the number and quality of your diffraction experiments, ensuring your success in increasingly competitive funding and IP environments.

LAB IN THE SPOTLIGHT



The new XtaLAB Synergy-S at Howard University. Tim Ramadhar (left) and Ray Butcher (right).

A major research thrust for Professor Tim Ramadhar's group involves the further development and application of the crystalline sponge method. Some of the aspects of this method that are being studied in his laboratory group include sponge growth, inclusion techniques, generation of new frameworks, and computationally probing crystalline sponges using quantum-chemical calculations. He has an active collaboration with Pfizer Inc.

Ray Butcher's research focuses on the structural chemistry of both organic and inorganic compounds. For organic compounds, several of the projects involve determining the structures of pharmaceutically active compounds. For inorganic compounds, projects include determining the structures of spin-crossover molecules, molecular magnets, and metal complexes with ligands based on Schiff bases of amino acids.

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BOOK REVIEW



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.



By David Quammen ISBN: 9781982164362

David Quammen's *Breathless: The Scientific Race to Defeat a Deadly Virus* is not the first work of popular science nonfiction to come out of the SARS-CoV-2 pandemic, and certainly will not be the last. However, it is an intriguing perspective on a global viral disaster, the ramifications of which will be felt for many years to come. Quammen boldly tackles these recent events, weaving a vivid tapestry of living history across continents, crafting a narrative that is easy for any layman to follow.

Quammen begins with an open and honest author's note, informing readers that, unlike his other works, this book—like much of the work done during the COVID-19 pandemic—was researched over Zoom. He also notes that he preserved the integrity of all his interviewees' quotes, even in cases where that might introduce grammatical errors or some inconsistencies in language. He claims to have done so out of respect for the truth, and the result is a story that has a tangible humanity. Every expert researcher and public figure feels much more like a real person with a voice and a personality with whom one could have a conversation, not just a figurehead in a position of authority generating a quote.

One would be hard-pressed to find someone on the planet who has been alive for the past three years and not been touched by the coronavirus pandemic. Whether they've gotten sick themselves, or lost a loved one to the disease, or their employment has been compromised, or their entire livelihood been at risk or lost, everyone has a COVID-19 story. Quammen's approach to documenting the race around the globe to identify, vaccinate against, and hopefully eradicate this disease is everaware of that sensitivity, that this is not a thing of the past—this is a very real, and in many ways very traumatic worldwide phenomenon.

Breathless, however, isn't just about COVID-19. It includes a broader series of snapshots in history, including earlier SARS, avian flu and swine flu epidemics. As a world, our scientific understanding of how the coronavirus transmits and replicates comes from decades of research and experience with other diseases. Quammen makes sure to interweave these relevant contexts into the broader narrative of COVID-19 when necessary. The result is deeply compelling.

In some ways, *Breathless* is reminiscent of Richard Preston's *The Hot Zone*, a 1994 nonfiction book about viral hemorrhagic fevers, such as Ebola. *Breathless* is less of a chilling thriller than Preston's work, which it needs to be in order to be tactful, given the ongoing nature of the pandemic. However, it is just as fast-paced and quick to read, each short chapter giving way to the next, until you realize you've hit the credits which are extensive. Quammen takes the time to provide a brief blurb for every single person he interviewed while writing the book, including information about the date of the interview, what they discussed, and their professional background.

Jeanette S. Ferrara, MFA





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