CRYSTALLOGRAPHY TIMES

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WELCOME

I woke up a couple of weeks ago to a poem initiated by Eddie Snell from the Hauptman-Woodward Medical Research Institute and produced by ChatGPT.

Here it is:

In the world of X-ray diffraction,
Rigaku reigns supreme,
A beacon of precision,
Instruments beyond our wildest dream.

From crystals to powders,
Rigaku does it all,
No sample too complex,
No challenge too tall.

With detectors and software,
Their systems are complete,
From the lab to the field,
Their technology can't be beat.

Innovation is their hallmark,
Their dedication clear,
With Rigaku by our side,
We have nothing to fear.

So here's to Rigaku,
A leader in crystallography,
Their impact on science,
Is a true legacy.

In the spirit of the Japanese origin of Rigaku, I asked for a haiku and got:

Rigaku's X-rays reveal,
Nature's secrets held.

I don't know about you, but I find these amazing, in the sense that these are better than any poetry I could produce (although it didn't get the haiku structure right). I am not worried about sentience, yet. Try this on other entities and you'll find similar patterns. What I have found ChatGPT useful for is distilling relatively old (from 2020 or earlier) information into an understandable format. It is not perfect, but I am finding it more useful than Google or the old Bing.

This month we highlight the laboratory of Professor Tasos Tasiopoulos at the University of Cyprus and CrysAlis^{Pro}'s AutoChem plugin. There was a dearth of single crystal diffraction papers in the news, so I've picked a couple of papers on differing methods for solving the dynamical diffraction problem for electrons. I did see a very interesting paper on a close-to-ambient conditions superconductor and include it even though the authors used powder XRD in their characterization of the material.

The war in Ukraine is now in its second year. So that we do not forget this, the useful link provides information on helping relief efforts in Ukraine.

This month's video of the month is a celebration of the 50th Year of MiniFlex production. Finally, *Jeanette reviews Tesla: Wizard at War: The Genius, the Particle Beam Weapon, and the Pursuit of Power.*

Be safe,
Joe

RESE LAB TOUR DURING DGK

Please join us for a lab tour during DGK this March. The tour will be on Thursday 30th March from 2pm, 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.

PRODUCT IN THE SPOTLIGHT

Automated Structure Determination Plugin AutoChem

When it is in online mode, AutoChem performs fully automatic structure determination and refinement during data collection. It automatically processes every 25 frames, reduces data, updates the *.hkl, *.ins and *.cif_od files and determines and refines the structure. Users can confirm the results of structure determination even during data collection. AutoChem is an automatic structure analysis program in a narrow sense but, in a broad sense, it involves seamlessly from diffraction image collection to structure determination and it can give feedback and show results in real time during data collection. AutoChem automatically selects multiple optimal programs (direct methods (SHELXT, SIR), the Patterson method and the charge-flipping method) to maximize the success of structure determination. Users are also able to solve and refine structures interactively using Olex^2, as well as make custom reports.

Online mode

After 75 frames, data processing runs simultaneously with diffraction image collection.
The following data processing steps run automatically after every 25 frames:

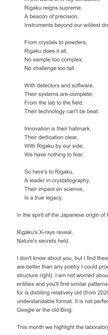
- Data reduction
- Update *.hkl, *.ins and *.cif_od files
- Structure determination and refinement

- The optimal program is chosen automatically to maximize the probability of solving the structure, from among direct methods (SHELXT, SIR), Patterson methods and charge-flipping methods
- Users can manipulate and fine-tune the structure interactively using Olex^2
- Reports can be easily generated

LAB IN THE SPOTLIGHT

Professor Tasos Tasiopoulos (right) is shown here with his freshly installed XtaLAB Synergy-S and our service engineer, Keith Fallon-Norris, responsible for the installation. His new instrument joins a 10-year old Supernova in his lab at the University of Cyprus. Professor Tasiopoulos has been lecturing at the University of Cyprus in the Chemistry department since 2004 following completion of a postdoc position at the University of Florida under Prof. George Christou. His studies focus on stereochemistry, integrating crystal analysis structure and medicinal chemistry. He also has research projects in supramolecular chemistry and ground state analysis of metallic clusters.

BOOK REVIEW



Review: *Tesla: Wizard at War: The Genius, the Particle Beam Weapon, and the Pursuit of Power*
By Marc J. Seifer
ISBN: 9780806540986

Tesla: Wizard at War: The Genius, The Particle Beam Weapon, and the Pursuit of Power is an intriguing deep dive into the intersection of inventor and engineer Nikola Tesla's career and the advent of modern warfare and the race to develop cutting-edge military technologies.

It is not about the infamous "Current War" between Tesla and Thomas Edison regarding whether the use of alternating current or direct current is safer for delivering electrical energy to the masses. The "War" Seifer is referring to in his title is literally World Wars I and II. If anything, *Wizard at War* seems to downplay the rivalry between Tesla and Edison, suggesting that Edison's support of Tesla when he needed a space to conduct his research indicates something almost akin to a comradery between the two famous scientists.

Seifer refers to his 1996 biography of Tesla, titled *Wizard: The Life and Times of Nikola Tesla*, several times. *Wizard at War* is less of a traditional biography in several senses. It is not a strictly chronological narrative; at times, Seifer bounces back into Tesla's past as it provides meaningful context to the narrative, but it is by no means a complete biography of Tesla's entire life. It also reads a bit like a historical mystery, as Seifer is working with primary source letters and notes from Tesla's myriad correspondences in his later career. One gets the sense, even without having read it, that *Wizard* is a more customary biography of Tesla's life, from early childhood to death, whereas *Wizard at War* focuses on a singular period in Tesla's life in which he sought to develop a teleforce weapon labeled a "death ray" by the press at the time.

Tesla claimed, at the time of his death, that had managed to build and experiment with an actual particle beam weapon. *Wizard at War* is Seifer's well-researched and methodically sourced investigation into whether Tesla's claim was founded in fact. Seifer pieces together evidence ranging from interviews with veterans who remember meeting Tesla to letters and notes sent to his various professional and personal connections. Seifer also includes a detailed dissection of the Trump Report, a dossier compiled by the United States government following Tesla's death meant to summarize the country's investigation into the validity of Tesla's claims.

To divulge any more would perhaps ruin the plot—although it is all, of course, merely history.

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 watch recordings our past sessions here.

UPCOMING WEBINAR

TOPIQ | The New ACTOR 2 Sample Changer for Automating your Single Crystal Workflow.
Wednesday, April 26, 2023.

UPCOMING EVENTS:

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

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

GCCW23, 14th Canadian Chemical Crystallography Workshop, Vancouver, Canada, May 30-June 3, 2023

CSC 2023, Canadian Chemistry Conference and Exhibition, Vancouver, Canada, June 4-8

CRYSTALLOGRAPHY IN THE NEWS

Cleverley and Beanland describe a Bloch-wave approach to the dynamical diffraction problem by modeling electron diffraction data with dynamical Bloch-wave simulations.

Drevon, Waterman and Krissinel describe an alternate method to the dynamical diffraction problem by applying the T-matrix approach to the solution of Schrödinger's equation.

Researchers from the University of Rochester and Unearthly Materials, Inc. report evidence of near-ambient superconductor in a nitrogen-doped lutetium hydride.

USEFUL LINKS

It has been just over a year since Russia invaded Ukraine. This link is a year old but still provides useful information regarding relief efforts for Ukraine: Here's how you can help the people of Ukraine - NPR

VIDEO OF THE MONTH

The MiniFlex was introduced in 1973 as the world's first benchtop X-ray diffractometer. It recorded X-ray intensity on a chart recorder. Since then, the MiniFlex has undergone generations of improvements based on customer feedback and support. Along the way, users have published over 43,000 papers and patents and let the MiniFlex be part of it. Here is a short video celebrating the 50th Year of the MiniFlex.

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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9009 New Trails Drive, The Woodlands, TX 77381, United States