



CRYSTALLOGRAPHY TIMES

Volume 12, No. 10, December 2020

WELCOME

Good day everyone. COVID-19 vaccines are starting to roll out across the globe. An ICU nurse in New York was among the first people in the U.S. to receive the coronavirus vaccine, and the first person in the UK was a 91-year-old grandmother. The second person in the U.K., believe it or not, was an 81-year-old man named William Shakespeare! After a year where the pandemic has had such a profound worldwide impact and everyone has had to make adjustments, let's hope that this vaccine rollout is the first step toward making 2021 a better year.

We've just completed the Rigaku Advanced Topics in Practical Crystallography School. The school covered powder and PDF collection and analysis, high-pressure data collection and analysis, new features in CrysAlis^{Pro} and the new non-spherical atom refinement system NoSpherA2 in Olex2. We averaged about 200 students per day and look forward to seeing how well the students perform when we complete the exam later this week.

This month, our product in the spotlight is the Rigaku XtaLAB Synergy Flow, a perfect solution to social distancing and remote access research. Our researcher in the spotlight is Mike Katz from Memorial University of Newfoundland.

Our usual sections include a few noteworthy crystallography papers and one paper on protein folding that has the CCP4 BB abuzz. Our video links cover MicroED and XDSgui, while the useful links take you to two helpful COVID-19 sites. This month, Jeanette reviews *Anti-Vaxxers: How to Challenge a Misinformed Movement*, which should provide some lively discussion around the holiday table if you choose to visit family and friends.

I trust science,

Joe

CRYSTALLOGRAPHY IN THE NEWS

October 30, 2020: Researchers at Ludwig-Maximilian University of Munich have [synthesized oxygen-rich bis \(trinitroethyl esters\)](#) that may provide safer alternatives to ammonium perchlorate in the area of solid rocket propellants.

November 18, 2020: Researchers at the University of British Columbia and Simon Fraser University determined the [structure of wild-type SARS-CoV-2 main protease acyl-enzyme intermediate](#) with a physiological C-terminal autoprocessing site, which provides insight into blocking the main protease.

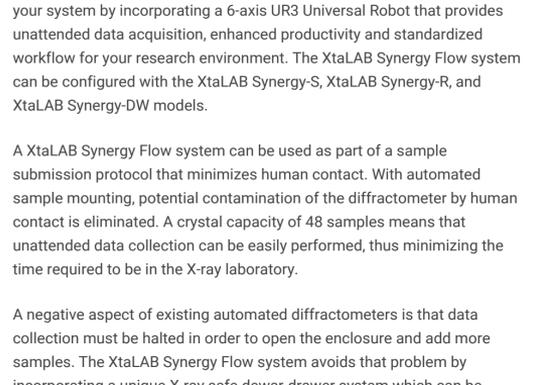
November 20, 2020: Researchers from Belgium, France, Italy, Switzerland and the U.S. used a crystal structure of a novel antibody to build a model of [ultrapotent human antibodies that protect against SARS-CoV-2](#) challenge via multiple mechanisms.

November 23, 2020: Chemists at the Chinese University of Hong Kong have [synthesized and characterized 15- and 16-vertex closo-carboranes](#), the first increase in vertex number since 2005.

November 30, 2020: The biggest news item this month is the press release from DeepMind and CASP-14 on the success of AlphaFold2, an AI for folding proteins *in silico*. Here is a [short analysis by John Helliwell](#). I also suggest reading the thread on the [CCP4 Bulletin Board](#) for a variety of opinions.

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy Flow: The Perfect Solution to Social Distancing and Remote Access Research



The XtaLAB Synergy product line has proven to be very popular for single crystal analysis. With the choice of a range of high-performance X-ray sources as well as direct X-ray detection detectors, there is a model of the XtaLAB Synergy to meet the needs of any researcher. The XtaLAB Synergy Flow system allows you to now take full advantage of the performance of your system by incorporating a 6-axis UR3 Universal Robot that provides unattended data acquisition, enhanced productivity and standardized workflow for your research environment. The XtaLAB Synergy Flow system can be configured with the XtaLAB Synergy-S, XtaLAB Synergy-R, and XtaLAB Synergy-DW models.

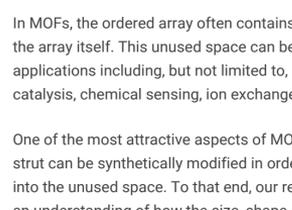
A XtaLAB Synergy Flow system can be used as part of a sample submission protocol that minimizes human contact. With automated sample mounting, potential contamination of the diffractometer by human contact is eliminated. A crystal capacity of 48 samples means that unattended data collection can be easily performed, thus minimizing the time required to be in the X-ray laboratory.

A negative aspect of existing automated diffractometers is that data collection must be halted in order to open the enclosure and add more samples. The XtaLAB Synergy Flow system avoids that problem by incorporating a unique X-ray safe dewar-drawer system which can be ejected from the side of the cabinet while data collection continues unimpeded.

The XtaLAB Synergy Flow system is the perfect solution to allow full time use of your diffractometer during a time when human interaction and contamination must be minimized.

RESEARCHER IN THE SPOTLIGHT

Michael J. Katz
Assistant Professor, Chemistry
Memorial University of Newfoundland



The Katz research program focuses on the synthesis, properties, and applications of porous materials. The porous materials they work with are being designed for various applications. For example, current porous materials research includes, but is not limited to, gas storage (e.g., low-pressure methane storage), chemical separation (e.g., removal of harmful molecules from air) and catalysis.

Metal-organic frameworks (MOFs) are porous materials. They are also a sub-class of coordination polymers in which organic molecules (*i.e.*, struts, linkers) are joined with metal cations (*i.e.*, inorganic nodes) to form an ordered array.

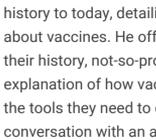
In MOFs, the ordered array often contains space that is not occupied by the array itself. This unused space can be used for a variety of applications including, but not limited to, gas storage and separation, catalysis, chemical sensing, ion exchange and drug delivery.

One of the most attractive aspects of MOF synthesis is that the organic strut can be synthetically modified in order to introduce new functionality into the unused space. To that end, our research team focuses on gaining an understanding of how the size, shape and functionality of the unused space relates back to the MOFs utility in various material properties.

Here is an example of a recent publication:

[Selective decontamination of the reactive air pollutant nitrous acid via node-linker cooperativity in a metal-organic framework](#), Devon T. McGrath, Michaela D. Ryan, John J. MacInnis, Trevor C. VandenBoer, Cora J. Young and Michael J. Katz, *Chem. Sci.*, 2019, **10**, 5576.

BOOK REVIEW



[Anti-vaxxers: How to Challenge a Misinformed Movement](#)
By Jonathan M. Berman
ISBN: 9780265239326

Jonathan M. Berman's *Anti-Vaxxers* is described on its cover as "the essential companion to inform conversations with family and friends," presumably about vaccination science, or rather, as the title suggests, those who choose not to believe in it.

Berman's preface speaks to the importance of vaccinations and the alarming threat of anti-vaxxers in the context of the current COVID-19 global pandemic. Though Berman clearly wrote the preface in the earlier days of the virus, many of his statements and concerns ring true even now, more than half a year in. One of the largest questions looming on the horizon will certainly be the response of anti-vaxxers to any COVID-19 vaccine to come on the market and, of course, any government declarations deeming vaccination mandatory.

Berman approaches the subject of vaccinations and those who call themselves anti-vaxxers broadly, and then winnows his way through history to today, detailing both the good and the bad information out there about vaccines. He offers his reader a better understanding of vaccines, their history, not-so-proud moments in their history, and an underlying explanation of how vaccines work. His clear goal is to provide his readers the tools they need to compose a compelling counter-argument when in conversation with an anti-vaxxer.

Berman's approach to anti-vaxxers is neither condescending nor disempathetic, but measured and informed. As he explains throughout the book, many anti-vaxxers are not uninformed but, rather, ill-informed. That is, they do not believe in vaccinations for their children and perhaps themselves not because they do not understand what vaccinations are or how they work, but rather because they have been exposed to, consumed and believed "fake news" regarding this medical practice.

One important thing to consider, which Berman certainly hammers home, is the importance of understanding what information is out there, and what is scientifically sound and what is not. Indeed, the infamous 1998 *Lancet* paper by Andrew Wakefield surmising that vaccinations caused autism spectrum disorder to develop in otherwise unaffected children is still cited today by anti-vaxxers aiming to support their stance. Yet the paper was retracted, and Wakefield stripped of his medical license in the United Kingdom for falsifying results.

Berman also explores the role of pop culture in public perception of vaccinations, from non-expert celebrity endorsements to ill-researched documentaries to falsely sourced articles published in popular magazines. It's important when speaking with an anti-vaxxer to understand where they are coming from and where the information they have may be coming from. There's a good chance it's either word of mouth or coming from someone who has no clinical or medical experience.

Setting aside the distinction between pseudoscience, falsified publications and real medical research, another important consideration is the history of vaccinations. It is fraught with blemishes, many of which resulted in numerous unnecessary deaths. There was the horse named Jim who was used to culture antitoxin for a vaccine that then killed its inoculants because, unbeknownst to the vaccine manufacturer, Jim had tetanus. Then there was the case of the polio vaccines that were incorrectly developed and actually gave people polio, several of whom died.

If Berman's book makes anything clear, it's that anti-vaxxers don't have solid legs to stand on in their arguments, but their arguments do have legs. There have been times when vaccines have failed to meet their intended purpose, being causing more harm than good. But, fundamentally, their success in eradicating terrible diseases such as polio, the measles and smallpox cannot be underwritten by their failure. And, most importantly, the fundamental basis of the modern anti-vaccination movement is the concern that there is a connection between childhood vaccinations and autism—a concern seeded by a nearly 25-year-old publication that has since been retracted, denounced and disgraced.

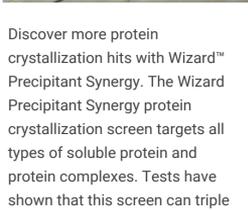
If you have any anti-vaxxers in your life, especially with the holidays coming up, you'll probably benefit from reading Berman's book.

Review 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.

RIGAKU REAGENTS



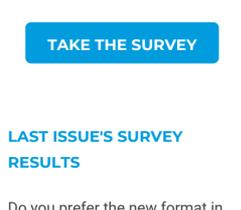
Discover more protein crystallization hits with Wizard™ Precipitant Synergy protein crystallization screen targets all types of soluble protein and protein complexes. Tests have shown that this screen can triple the number of unique crystals compared with other screens. Each unique formulation is made available in three different concentrations to increase the coverage of crystallization space. These related **formulations are positioned in neighboring wells or tubes to simplify the analysis of crystallization behavior**. This format creates less waste than the previous 64-well formats and it enables high-throughput crystallization, using 2x96=192 formulations in two crystallization plates, for initial protein crystallization screening and crystallization optimization.

Wizard Precipitant Synergy Tubes: 1009539
Wizard Precipitant Synergy Block: 1008652

[SHOP HERE](#)

SURVEY OF THE MONTH

Do you plan on being vaccinated for COVID-19 when a vaccine is made available to you?

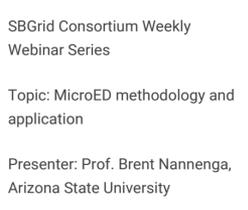


LAST ISSUE'S SURVEY RESULTS

Do you prefer the new format in which all content is displayed in the email or the older format in which all content was available as a PDF?



VIDEOS OF THE MONTH



Prof. Brent Nannenga - MicroED methodology and application

SBGrid Consortium Weekly Webinar Series

Topic: MicroED methodology and application

Presenter: Prof. Brent Nannenga, Arizona State University



XDS and XDSGUI

SBGrid Consortium Weekly Webinar Series

Topic: Crystallographic data processing with XDS, using XDSGUI

Presenter: Kay Diederichs, Professor, Universität Konstanz

USEFUL LINKS

[COVID-19 Projections](#)
The Institute for Health Metrics and Evaluation (IHME) is an independent global health research center at the University of Washington. This link provides projections by country.

[COVID-19 Indoor Safety Guideline](#)
This app, developed by [Kasim Khan](#) in collaboration with [Martin Z. Bazant](#) and [John W. M. Bush](#), uses a theoretical model to calculate safe exposure times and occupancy levels for indoor spaces. By adjusting room specifications, ventilation and filtration rates, face-mask usage, respiratory activities and risk tolerance (in the other tabs), you can see how to mitigate indoor COVID-19 transmission in different indoor spaces.

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.

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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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