



Volume 15, No. 6, June 2023

WELCOME

When this arrives in your inbox, we will be two weeks out from the ACA meeting in Baltimore and two months away from IUCr in Melbourne. I am fortunate that I will be able to attend both meetings and look forward to seeing many old friends at both. I hope that you will be able to make at least one of the meetings.

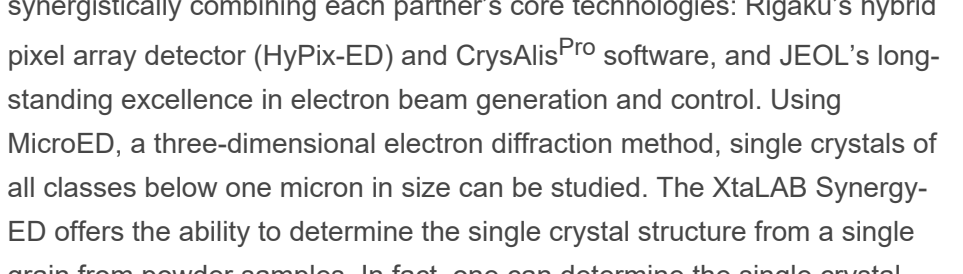
In other exciting news, we have installed the first XtaLAB Synergy-ED systems outside of Rigaku this past month, at ICIQ in Spain and at the University of Warwick in the UK. Before the year is out, we expect to install three more in Europe and one in the US.

This month we highlight the lab of Professor Kasper S. Pedersen at the Technical University of Denmark, who acquired the first XtaLAB Synergy-ED in Denmark. Our product in the spotlight is the venerable XtaLAB mini II benchtop X-ray diffractometer.

In addition to the usual monthly items, I would like to draw your attention to Jeanette's review of *Distrust: Big Data, Data Torturing, and the Assault on Science*.

Travel safely,
Joe

UPCOMING WEBINAR



The Rigaku XtaLAB Synergy-ED is a fully integrated electron diffractometer, with a seamless workflow from data collection to 3D structure determination. The XtaLAB Synergy-ED is the result of Rigaku's collaboration with JEOL, synergistically combining each partner's core technologies: Rigaku's hybrid pixel array detector (HyPix-ED) and CrysAlis^{Pro} software, and JEOL's long-standing excellence in electron beam generation and control. Using MicroED, a three-dimensional electron diffraction method, single crystals of all classes below one micron in size can be studied. The XtaLAB Synergy-ED offers the ability to determine the single crystal structure from a single grain from powder samples. In fact, one can determine the single crystal structure of multiple compounds present in a single powder sample.

There are two well-characterized polymorphs of acetaminophen with known single crystal structures. In this presentation, we will explore the case of a third polymorph of acetaminophen generated in an XRD-DSC experiment with a structure determined by MicroED. This result is a major step in understanding the properties of acetaminophen and demonstrates the potential to solve many more unsolved problems in structural science.

Date/time

Wednesday, July 19, 2023 09:00 AM CDT
[Register >](#)

PRODUCT IN THE SPOTLIGHT



XtaLAB mini II

Single crystal X-ray diffraction on your benchtop

The perfect addition to any synthetic chemistry laboratory, the XtaLAB mini II single crystal X-ray diffractometer will enhance research productivity by offering affordable structure analysis capability without the necessity of relying on a departmental facility. With the XtaLAB mini II benchtop diffractometer, you no longer have to wait in line to determine your structures. Instead, your research group can rapidly analyze new compounds as they are synthesized in the lab without having to queue up in the departmental core facility.

Teach single crystal X-ray diffraction through hands-on experience

In many universities, the departmental single crystal X-ray diffractometer is considered off limits to students because of fear the instrument might be damaged by inexperienced users. The XtaLAB mini II benchtop diffractometer provides the opportunity for students to learn single crystal X-ray analysis by actually using a fully functional diffractometer. This is not a black box instrument. Rather, performing the important steps of mounting a crystal on the goniometer and physically centering the crystal in the position of the X-ray beam ensures that students learn the importance of mounting techniques and crystal selection. The simple design of the XtaLAB mini II X-ray diffractometer minimizes the possibility of students misaligning or damaging the system.

Compact size with excellent X-ray data quality

The Rigaku XtaLAB mini II is a research-grade chemical crystallography diffractometer that sits on the benchtop. No data quality compromises. Results delivered are unambiguous. X-ray source tube lifetime is extended by running a standard off-the-shelf X-ray tube at 600 W. To compensate for running at a lower power, a SHINE optic (special curved monochromator) is utilized to produce usable X-ray flux comparable to a standard X-ray diffractometer. In addition, the XtaLAB mini II is equipped with a state-of-the-art two-dimensional semiconductor detector that is characterized by extremely low background noise and high sensitivity. These detector characteristics mean that, for weakly diffracting samples, longer scan rates can be employed without the weak diffraction signals being swamped by detector noise.

Dedicated to producing publication quality single crystal X-ray structures

The chief design requirement when creating the XtaLAB mini II single crystal X-ray diffractometer was that the structures produced would be publishable in the most demanding scientific journals. The HPC X-ray detector is positioned so that the maximum 2θ value is well outside of the Acta Cryst. requirements. The software provides all the tools you need to generate publication quality data that can be used to determine 3D structures from a variety of structure analysis packages.

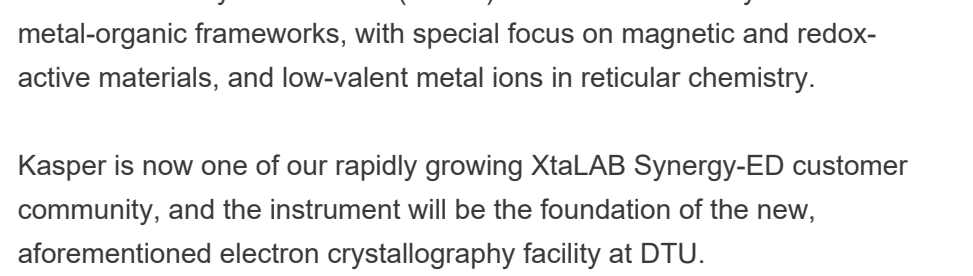
CrysAlis^{Pro} single crystal X-ray diffraction software

The XtaLAB mini II comes complete with CrysAlis^{Pro}, our user-inspired data collection and data processing software for single crystal analysis. Designed around an easy-to-use graphical user interface, CrysAlis^{Pro} can be operated under fully automatic, semi-automatic or manual control. CrysAlis^{Pro} combines automated crystal screening, the fastest and most accurate strategy software available, concurrent data reduction and automatic small molecule structure solution. Visual feedback is provided for each step with clear, color-coded guidance so that both novices and experts can collect high-quality data in the shortest time possible.

AutoChem: Automated single crystal structure determination software (optional)

AutoChem is an optional software package for the XtaLAB mini II and is the ultimate productivity tool for chemical crystallographers, offering fast, fully automatic X-ray structure solution and refinement during data collection. Developed in collaboration with OlexSys Ltd (Durham University, UK), AutoChem works in conjunction with Olex² where more advanced structure solution and refinement functionality exists. AutoChem is seamlessly integrated within CrysAlis^{Pro} and forms an integral part of our "What is this?" feature. The "What is this?" feature gives you structures quickly and ensures you are not wasting time collecting full datasets on known samples or starting materials. It is an convenient pre-experiment option, which is used to plan your full data collections.

LAB IN THE SPOTLIGHT



Professor Kasper Pedersen

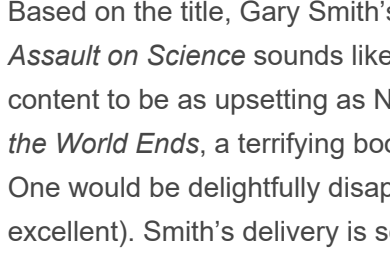
Professor Kasper Pedersen is professor of chemistry at the Technical University of Denmark (DTU) and, now, director of the DTU Electron Crystallography Facility due to be inaugurated later this year.

Kasper has been at DTU since 2017 following postdoctoral positions at the Centre de Recherche Paul Pascal (CNRS) and the Institute of Condensed Matter Chemistry of Bordeaux (CNRS). His research mainly involves metal-organic frameworks, with special focus on magnetic and redox-active materials, and low-valent metal ions in reticular chemistry.

Kasper is now one of our rapidly growing XtaLAB Synergy-ED customer community, and the instrument will be the foundation of the new, aforementioned electron crystallography facility at DTU.

We are both pleased and excited to contribute to this venture and look forward to seeing the publications start to flow.

BOOK REVIEW



Review: [Distrust: Big Data, Data Torturing, and the Assault on Science](#) By Gary Smith

ISBN: 9780192868459

Based on the title, Gary Smith's *Distrust: Big Data, Data Torturing, and the Assault on Science* sounds like nightmare fodder. One might expect the content to be as upsetting as Nicole Perle's *This is How They Tell Me the World Ends*, a terrifying book about the cutting edge of cyberwarfare. One would be delightfully disappointed (not that Perle's book isn't also excellent). Smith's delivery is so delicately and effortlessly enmeshed with endless dry wit that you might actually find yourself laughing out loud as you read it—surely to be followed by a deep frown as you contemplate the powerful implications of what he is saying.

Smith opens with an introduction in which he details two different kinds of currency: (1) rai stones, used only on the island of Yap in Micronesia, which have incredible value and (2) cryptocurrency, which is used worldwide and has no inherent value. Smith even draws comparisons between the current international fascination with cryptocurrency and mid-19th century America, when any bank could print money and it would get used even though it was counterfeit and had no financial guarantee of value. He uses these finance-based examples, among others, to illustrate the real-world implications of unethical data practices and how they sow distrust in scientific fact and the definition of truth in reality before digging deeper into disinformation, data torturing, and data mining.

Smith pins the current sociopolitical climate in which the general American populace seems to have little or no trust and/or faith in scientific reasoning on a combination of three prolific factors: (1) disinformation, the spread of information that simply isn't factual, (2) data torturing, manipulating large swaths of data to get low p-values, also known as p-hacking, and (3) data mining, collating large amounts of unrelated data and accounting correlation to causation to prove a theory posited after the data was collected. Smith dives into each of these pitfalls in each of the first three parts of the book.

In Part IV, Smith takes a relevant sidestep and dives into the world of artificial intelligence, which he boldly and wittily refers to as "artificial unintelligence." One unfortunate side effect of the fast pace with which technology is developed in our world is that, even though *Distrust* came out in June 2023, Smith was not able to include any insights into the recent rollout of OpenAI's Chat GPT-4 (he has lots of thoughts about Chat GPT-3's uselessness in the grand scheme of reality), nor into Google's recent rollout of Bard, one of the other more advanced AIs to become available in the first half of the year. Though his overall approach to analyzing the social value of AI in our recent past, our present, and our future is arguably still sound, it would have been intriguing to include an epilogue digging a little deeper into the most recent advancements.

Smith ends with Part V, "The Crisis," in which he re-outlines the thesis of his book as presented in the introduction, along with a concise yet comprehensive list of action items individuals, corporations, and governments can take to combat the war on science waged by widespread disinformation, data torturing, and data mining. The chilling theme throughout *Distrust* is that science and those who pursue it are to some extent to blame for engaging in these practices that have led to public distrust in the first place.

Each chapter of *Distrust*, including the introduction, ends with a section titled "Irony," where Smith explains how the very technologies created to imbue the world with knowledge are empowering people not to believe in the science that powered their inventions. *Distrust* itself is not a work of satire but, given the breadth of historical examples Smith presents and the sheer ridiculousness of data abuse covered, at times it feels like it could be.

Distrust is a must-read for anyone with an interest in data, a concern for society, and/or a passion for science.

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 and electron diffraction, X-ray fluorescence and X-ray imaging. You can watch recordings of our past sessions [here](#).

UPCOMING EVENTS:

ACA 2023, 73rd ACA Annual Meeting, Baltimore, MD, July 7-11, 2023.

DXC 2023, Lombard, IL, August 7-11, 2023,

ACS Fall 2023, San Francisco, CA, August 13-17, 2023.

Rigaku European Single-Crystal Users' Meeting, Warwick University, UK, September 11-12, 2023.

IUCr 2023, 26th Congress and General Assembly of the International Union of Crystallography, Melbourne, Australia, August 22-29, 2023.

80th Pittsburgh Diffraction Conference, Pittsburgh, PA, October 15-17, 2023.

SERMACS 2023, Durham, NC, October 25-28, 2023.

Rayons X et Matière 2023, Bordeaux, France, November 21-24, 2023.

CRYSTALLOGRAPHY IN THE NEWS

May 8, 2023

Scientists in Australia have synthesized and characterized a novel magnesium reagent that will defluorinate poly(tetrafluoroethylene) at room temperature.

May 23, 2023

Researchers from the Max Planck Institute have synthesized and characterized a triplet bismuthinidene with a quenched magnetic response.

May 24, 2023

Scientists from the UK and US have discovered a small molecule activator for the kinase PI3Kα, which confers cardioprotection during reperfusion therapy and neuroregeneration after crush injuries.

June 7, 2023

Researchers from China have synthesized and characterized organic-inorganic covalent-ionic molecules displaying elastic, ceramic and plastic behavior concurrently.

USEFUL LINKS

In addition to the war in Ukraine, we have another humanitarian crisis in Sudan. It seems that medical aid is the most critical need now. [Doctors without Borders](#) is a reputable organization and is providing aid in Sudan.

Here is a link that provides useful information regarding relief efforts for Ukraine: [Here's how you can help the people of Ukraine: NPR](#)

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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.

[JOIN HERE](#)

