Volume 16, No. 3, March 2024

I just returned from an IUCr Finance Committee meeting and one of the topics we discussed was the Associates Programme. For a relatively small fee, one gets four major benefits: (1) a 20% discount on the publishing fee for an article in an open-access IUCr Journal, (2) six free downloads of articles from Crystallography Journals Online, (3) a 50% discount on individual price of print copies of *International Tables for Crystallography* (for personal use), and (4) discounts on books from the IUCr and other publishers such as Wiley, CRC Press and Elsevier. I have been an associate since the program's inception and highly recommend it.

This month we celebrate Mark Benson's promotion to Head of Single Crystal Business at Rigaku, a recognition for years of success in his time at Rigaku. We also highlight the XtaLAB Synergy-ED in the product spotlight. Christian Göb from RESE discusses the gnomonic projection and how to use it in the tip of the month. Jeanette reviews *The Einsteinian Revolution: The Historical Roots of His Breakthroughs* by Hanoch Gutfreund and Jürgen Renn.

Be safe,

Joe Ferrara

TOPIQ | High-pressure Crystallography on the Rigaku XtaLAB Synergy-S Diffractometer

In this Webinar, the process of conducting a high-pressure crystallographic experiment on the XtaLAB Synergy-S will be explained and software features in CrysAlis^{Pro} relevant to the technique will be covered. High-pressure crystallography provides a tool for researchers to effect changes in the structure of matter and ultimately understand the phenomena such changes can induce.

Friday, March 22, 2024 at 09:00 CST
Time Zone Converter

REGISTER NOW

Mark Benson has been appointed Head of Single Crystal Business at Rigaku

Mark joined Rigaku UK in 2005 following the completion of his PhD in Inorganic Chemistry at the University of Liverpool, where his research led to numerous crystal structures, fostering a deep appreciation of crystallography.

Commencing his Rigaku journey as a Sales Engineer, Mark transitioned from overseeing European territories to embracing more expansive global roles, rendering him a recognizable figure within the community.

Located in Chester, UK, he is in close proximity to the International Union of Crystallography and always happy to meet crystallographers visiting IUCr HQ.

"I'm extremely proud to work with an amazing group of talented people at such an exciting time for Rigaku Single Crystal business."

Rigaku UK team at the ECM in Marrakech in 2007, the one when our booth got stuck in customs for the entire event!

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy-ED

- Fully integrated electron diffractometer creating a seamless workflow from data collection to structure determination of three-dimensional molecular structures.
- Improve your ability to investigate nanocrystalline samples due to the ability of electron diffraction to measure crystals that are only a few hundred nanometers or less in size.
- No Sharing of instrument with microscopists because switching a microscope configuration between imaging and diffraction can be time consuming, making the sharing of an instrument sometimes difficult.
- Any X-ray crystallographer will find it intuitive to operate without having to become an expert in microscopy.

XtaLAB Synergy-ED is a new and fully integrated electron diffractometer, creating a seamless workflow from data collection to structure determination of three-dimensional molecular structures. The XtaLAB Synergy-ED is the result of an innovative collaboration to synergistically combine our core technologies: Rigaku's high-speed, high-sensitivity photon-counting detector (HyPix-ED) and state-of-the-art instrument control and single crystal analysis software platform (CrysAlis^{Pro} for ED), and JEOL's long-term expertise and market leadership in designing and producing transmission electron microscopes. The key feature of this product is that it provides researchers an integrated platform enabling easy access to electron crystallography. The XtaLAB Synergy-ED is a system any X-ray crystallographer will find intuitive to operate without having to become an expert in electron microscopy.

The XtaLAB Synergy-ED was designed to address the increasing need to investigate smaller and smaller samples in structural research. With X-ray crystallography, the smallest possible crystal dimension is 1 micron, and only then when utilizing the brightest X-ray sources and noise free detectors. However, in recent years, there has been an increasing need for the structure analysis of substances that only form microcrystals, crystals that are only a few hundred nanometers or less in size. In recent years, a new analytical method, MicroED, has been developed that uses electron diffraction on a TEM electron microscope to measure 3D molecular structures from nanocrystalline materials. Researchers developing this technique have relied on customized electron microscopes and a combination of microscopy software for measuring diffraction data, and public domain X-ray crystallography software for data processing and structure determination. Switching a microscope configuration between imaging and diffraction can be time-consuming, making the sharing of an instrument sometimes difficult.

To address these issues, Rigaku and JEOL started a collaboration to develop a dedicated single crystal structure analysis platform for nanocrystals utilizing key technologies from both companies. The result is the XtaLAB Synergy-ED, a dedicated electron diffractometer that is operated by the same control software that is used to run Rigaku's X-ray diffractometers and includes a complete integrated pipeline from sample selection and diffraction measurement to data processing and structure solution. This instrument can easily be installed in an existing X-ray crystallography facility, where researchers and students will be able to easily master the MicroED technique since the software workflow is the same as for an X-ray diffractometer. Having such an instrument installed in an X-ray facility immediately provides structure determination for materials that only form nanocrystals.

ACA SUMMER COURSE 2024

It is with great pleasure that the organizers of the ACA Summer Course announce the 2024 ACA Summer Course in Chemical Crystallography. The course will be held at Purdue University from June 23-30, 2024. For more details, please check the web page at https://acasummercourse.net/

Applications for the course are now open.

For international attendees requiring a visa to enter the United States: There have 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

The Organizers
Allen Oliver (University of Notre Dame), aoliver2@nd.edu
Matthias Zeller (Purdue University), zeller4@purdue.edu
Christos Malliakas (Northwestern), c-malliakas@northwestern.edu
Charlotte Stern (Northwestern), c-stern@northwestern.edu
Nathaniel Barker (Northwestern), nathaniel.barker@northwestern.edu

CRYSTALLOGRAPHY IN THE NEWS

February 8, 2024
Chemical and Engineering News published an article about Naica's crystal cave in Mexico.
February 13, 2024
Researchers from Australia and China synthesized and characterized a charge-neutral cryptand that selectively binds strongly hydrated sulfate anions in water.
March 6, 2024
Physicists from Canada, the UK and the US suggest buoyant crystals halt the cooling of white dwarf stars.
March 11, 2024
Also in *Chemical and Engineering News* was a news article describing how crystallography databases hunt for fraudulent structures.

TIP OF THE MONTH

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The Gnomonic Projection and How to Use It

What is the issue?
During long exposures on weakly scattering samples, inelastic scattering may contribute noticeably to the diffractogram, making unit cell indexing challenging. This scattering may come from the sample holder and oils used to mount the sample or air scattering. Electron diffraction may also exhibit inelastic scattering signals from the carbon support of the TEM grids. A human eye might find periodicity in a crowded reciprocal space more efficiently than a computer algorithm—for now.
How to find the unit cell of the crystal?
In the polar zenithal gnomonic projection, all difference vectors between reflections are calculated, normalized, and projected onto a plane tangential to the Ewald sphere. These difference vectors appear as individual pixels in this projection and a line is formed when these vectors appear in a periodic manner; e.g., they are equally spaced and parallel.

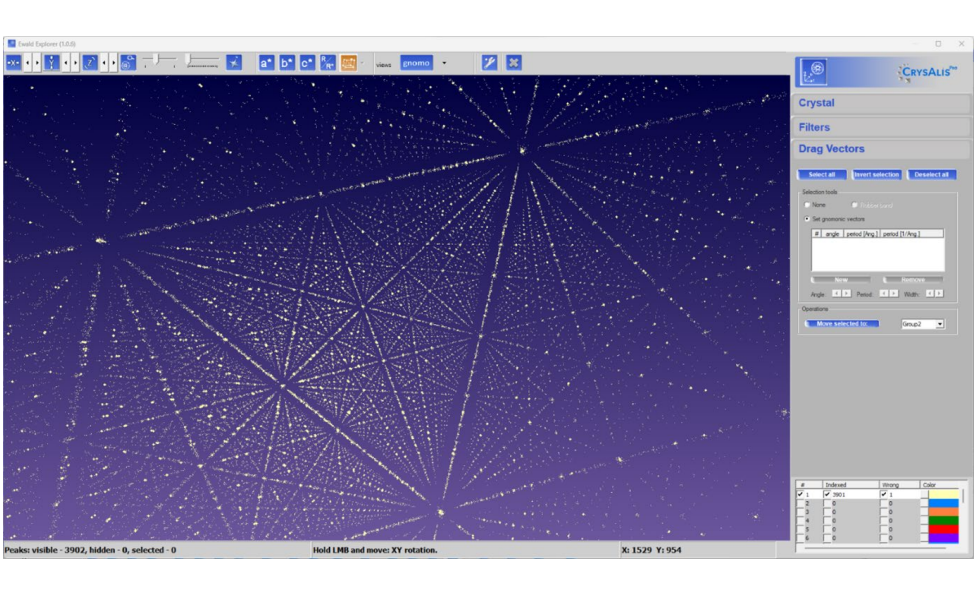


Figure 1. Gnomonic projection of the difference vectors in reciprocal space.

The task of the user is now to define three of these lines by choosing "Set gnomonic vectors." These lines cannot intersect each other at a single point and cannot be parallel. Figure 2 shows a histogram of the chosen reciprocal space direction. The abscissa shows the distance from the origin of reciprocal space and the ordinate shows the frequency at which the projected peaks appear.

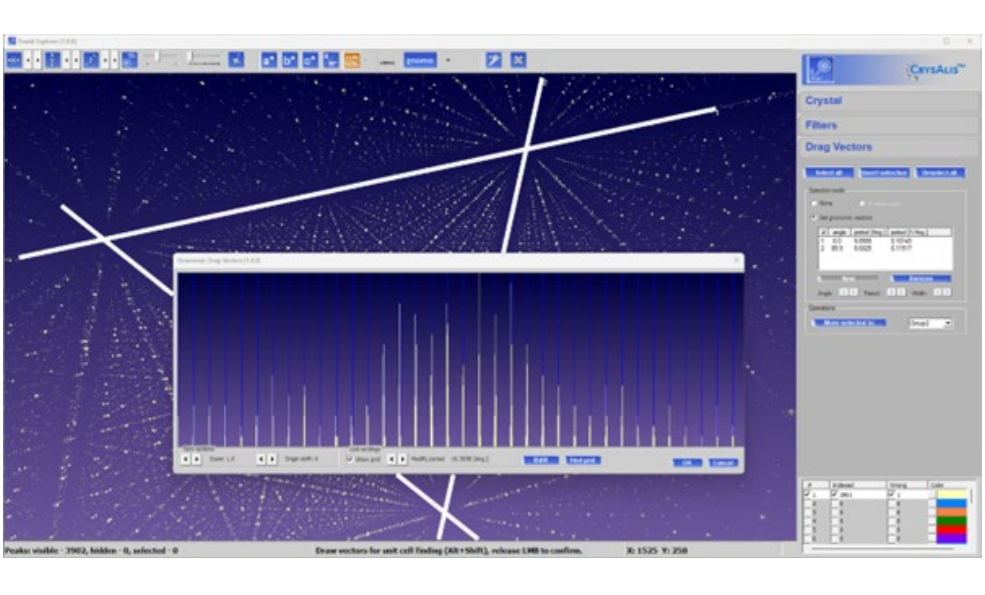


Figure 2. Three independent gnomic vectors set.

In the next step, we are presented with the lattice reduction, and we choose the one with the most meaningful G6-projection distance; see Figure 3. Further information can be obtained here: B. Gruber, *Acta Cryst.* (1973), **A29,** 433-440.

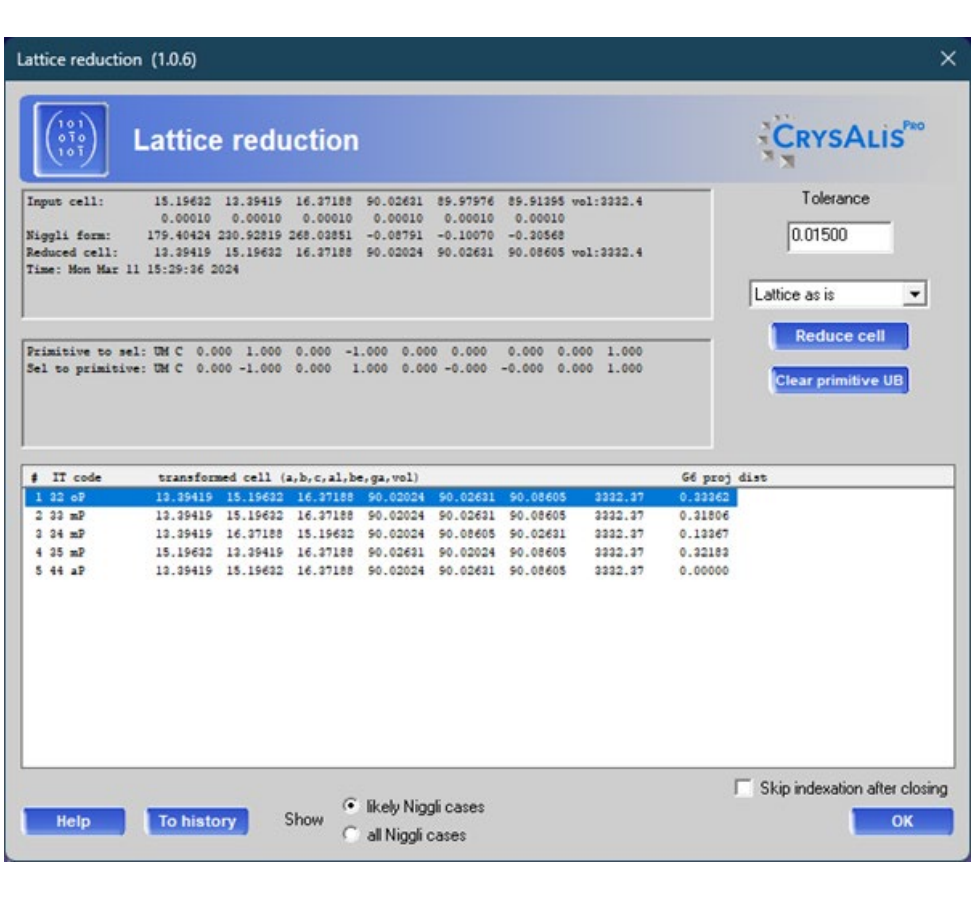
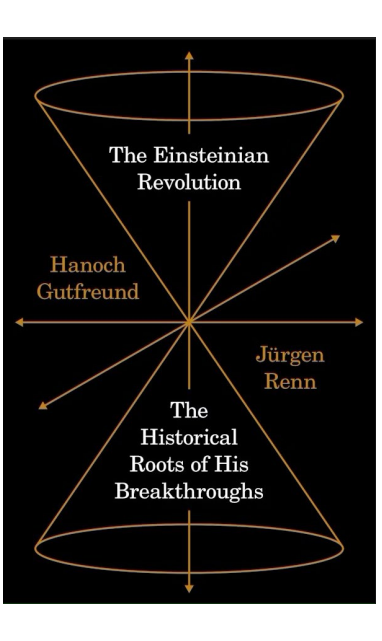


Figure 3. Lattice reduction with the most likely Niggli cases.

Acknowledgements
We thank Dr. Wolfgang Herrendorf (Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University Gießen) and STOE & Cie GmbH for the inspiration and fruitful discussions in creating this tool.

BOOK REVIEW



Review: *The Einsteinian Revolution: The Historical Roots of His Breakthroughs*
By Jürgen Renn and Hanoch Gutfreund
ISBN 9780691168760

Hanoch Gutfreund and Jürgen Renn's *The Einsteinian Revolution: The Historical Roots of His Breakthroughs* is not really about Albert Einstein at all. That is a good thing. There are too many books about Einstein when you take into account the dearth of good biographies about thousands of other influential scientists and mathematicians, including those whose research and ideas influenced Einstein.

In *The Einsteinian Revolution,* Gutfreund and Renn acknowledge that this plethora of biographical material has perpetuated an unfortunate and inaccurate narrative, one that paints Einstein as a lone genius, light years ahead of his colleagues in the world of physics. Rather than add to the heap, the authors offer an entirely different sort of narrative–one that purposely excludes Einstein for the most part.

Gutfreund and Renn don't exclude Einstein entirely–he gets a little biographical background, in case the reader really doesn't know who he is or where he came from or what he contributed to our understanding of modern physics. But most of the book explores the research and ideas that underlay the foundation of Einstein's theory of general relativity–the book's titular revolution.
Like Isaac Newton, if Einstein saw further, it was by standing on the shoulders of giants (including the shoulders of Isaac Newton himself). Gutfreund and Renn highlight the advancements in experimental and theoretical physics that made Einstein's so-called revolution possible–and the scientists who made these advancements..

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 and electron diffraction, X-ray fluorescence and X-ray imaging. You can watch recordings of our past sessions here.

UPCOMING WEBINAR:

TOPIQ | High-pressure Crystallography on the Rigaku XtaLAB Synergy-S Diffractometer
Friday, March 22, 2024
at 09:00 CST

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Register now >

UPCOMING EVENTS:

ACS Spring 2024, March 17- 21, 2024, New Orleans, LA

32nd Annual Meeting of the German Crystallographic Society (DGK), March 18-21, 2024, Bayreuth, DE.

BCA Spring Meeting, March 25-28, 2024, Leeds, UK.

2024 ACA Summer Course in Chemical Crystallography at Purdue University from June 23-30, 2024.

American Crystallographic Association Annual Meeting, July 7-12, Denver, CO

Denver X-ray Conference, August 5-9, Denver, CO

European Crystallographic Meeting 34, August 26-31, Padova, Italy

Second meeting of the Latin American Crystallographic Association (LACA), October 23-27, Mérida, Mexico

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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.

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.

JOIN HERE