Volume 16, No. 2, February 2024

The pollen is starting to fall here in southeast Texas, meaning spring has sprung. For those of you in the northern climes, you'll just have to wait a little longer. When we first moved here, in 1988, the pollen began falling in March not February. Hmmm, I wonder why it is so much earlier now…

This month we're taking the opportunity to introduce our newest Sales Manager, Josh Morris, who will take over James Gordon's territory. James has moved to the US from the UK and will have the eastern US and Canada as his territory. I am jealous—James has relocated to Maine—a wonderful place.

Our product in the spotlight is the recently updated IGH2, a motorized goniometer head with automated optical and X-ray object centering. Pierre Le Maguerès provides a tip for forcing a user-defined lattice for processing in CrysAlis^{Pro}. Jeanette reviews *Our Moon: How Earth's Celestial Companion Transformed the Planet, Guided Evolution, and Made Us Who We Are* by Rebecca Boyle.

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.

Wednesday, March 7, 2024 at 09:00 CST
Time Zone Converter

REGISTER NOW

INTRODUCING OUR NEWEST SALES MANAGERS

James Gordon, Regional Sales Manager, Eastern USA and Canada, at his new home in Maine.

My academic journey began at the University of Manchester, where I pursued a PhD focused on protein and nucleic acid biochemistry. Following my doctoral studies, I embarked on post-doctoral positions in various locations, including Boston, USA, Barcelona, Spain, and Cambridge, UK. These experiences provided me with a solid foundation in molecular and structural biology, broadening my perspective on research methodologies.

Transitioning into the field of sales was a natural progression for me. I started my sales career at Molecular Dimensions, supplying protein X-ray crystallographers with essential tools for their research. This role sparked my interest in sales and laid the groundwork for subsequent positions in the industry.

I then moved on to become Sales and Marketing Director for the consumable manufacturer SWISSCI, where I also managed the distribution of imaging systems designed to detect protein crystals. This role allowed me to further develop my skills in sales strategy and product marketing.

Continuing my career path, I took on the challenge of high-end instrument sales here at Rigaku, initially in Europe, covering territories across the UK, Scandinavia, the Middle East, and Africa. During this time, I played a significant role in facilitating sales of innovative technologies, such as the recently launched XtaLAB Synergy-ED electron diffractometer.

Despite being content with my role in Europe, my family and I were offered an exciting new opportunity by Rigaku to relocate to the USA. Recognizing the potential for growth and adventure, we enthusiastically embraced this new chapter. We chose Maine as our home. While the adjustment has presented challenges, we've found comfort in the familiar cold winter weather reminiscent of my UK roots, along with the welcomed addition of more sunshine and snow.

I'm now eager to embark on my latest role as Sales Manager for single crystal products in the Eastern region of the USA and Canada, representing Rigaku's offerings. I look forward to connecting with the scientific community, building relationships, and contributing my expertise to our shared objectives.

Joshua Morris, Sales Manager Single Crystal.

My academic career both started and ended at Cardiff University, with a brief one-year position at the University of Sydney in between. Studying initially for my Master's degree with Dr. Timothy Easun, I focused on the development of photoresponsive metal-organic frameworks and flexible organic ligands.

Having first become interested in crystallography as a Master's student running MOF single-crystals at Diamond Light Source, I moved on to conducting my PhD at Cardiff University under the supervision of Dr. Lauren Hatcher, focusing on the in-situ photocrystallographic investigation of hybrid perovskite materials. This has given me a fairly wide range of experience with both organic and inorganic framework materials, as well as a thorough background in single crystal X-ray crystallography, including several non-ambient in-situ methods. My primary research interest lies in the use of in-situ SCXRD to elucidate structure:function relationship in functional photoactive materials.

I then moved directly from the last stages of my PhD to Rigaku, into the role of Sales Manager for SCX across the EMEA regions, taking over from Dr. James Gordon as he moves to Rigaku America. I recognized how great an opportunity this has been, having been aiming to move into a sales position post-PhD.

My first few weeks on the job have been fascinating and a great introduction to the role, having visited several countries already for conferences and to facilitate sales in both X-ray and electron diffraction. I was lucky enough to benefit from James' wealth of experience in the first couple of weeks and utilized this to springboard into the role after some initial joint visits and calls. I'm excited to be working for Rigaku and looking forward to meeting and getting to know many of you in the coming weeks and months.

PRODUCT IN THE SPOTLIGHT

Intelligent Goniometer Head 2 (IGH2)

Benefits

- Automatic X-ray centering
- Reliable automated sample centering using optical object centering
- Hands-free, closed cabinet centering
- Minimized collision zone
- Use your existing mounts
- Centering in as little as 6 seconds

MOTORIZED GONIOMETER HEAD WITH AUTOMATED OPTICAL AND X-RAY OBJECT CENTERING

A minimal profile, automated goniometer head with built-in intelligence

Intelligent Goniometer Head 2 (IGH2)

Rigaku first offered a motorized goniometer head for the home lab, the Microglide, in 2004. Used both on Rigaku home lab instruments and on many synchrotron beamlines around the world, the Microglide was instrumental in changing the way cutting edge crystallography was performed. Today many beamlines operate in a hands-free way with users safely separated from the dangerous X-ray beam. The IGH2 is the successor to our popular IGH and has been engineered for the highest reliability, accuracy and precision with a major goal of significantly reducing the bulk compared with existing solutions. The IGH2 manages to further reduce the size compared to IGH and the end result is the smallest detachable motorized goniometer head on the market which gives you convenience, safety and automation possibilities with the minimum impact on data collection strategies.

AUTOMATED X-RAY CENTERING

Now with encoded motors inside, the IGH2 expands on the capabilities of its predecessor with automated X-ray centering. The goniometer performs scans at different grid points in order to reliably determine the point where the highest diffracted intensity is observed. X-ray centering is assisted by optical information to minimize scanning time.

AUTOMATED OPTICAL OBJECT CENTERING

For any truly automated system, reliably getting the sample centered in the X-ray beam without user input is essential. While older approaches used basic loop centering, or scanning through the X-ray beam, the IGH2 uses the latest in optical image recognition techniques to detect sample holder presence, recognize the crystal and center, not just the loop, but objects found within them. This fast approach minimizes dead time and avoids use of X-rays on sensitive samples and allows unattended data collection of an entire queue of samples when used in conjunction with a sample mounting robot like the ACTOR 2 system.

POINT & CLICK CENTERING MANUAL CONTROL

For a more manual approach, click on whatever you want to bring to the center of the goniometer and the IGH2 will move it into the beam. The IGH also allows fully manual movements for fine- tuning centering or handling more unusual cases.

BUILT-IN MAGNETIC MOUNT

For compatibility with commonly used sample mount standards including SPINE and ALS the IGH2 comes with a built-in magnetic mount. Such mounts are commonly used by both small molecule and macromolecular crystallographers and automated systems such as the ACTOR 2 system for automatic sample mounting. Conveniently, integrating the magnet also helps keep the size of the IGH2 to an absolute minimum.

SINGLE OR DUAL CAMERA OPERATION

Should you have an instrument supplied with dual video microscopes, the IGH is able to take advantage of both of them for faster centering without the need for rotations to get extra images. This allows centering to be completed typically within only 29 seconds. In a single camera setup, all that's needed is a simple 90° phi rotation to get all the visual information needed.

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 opened on January 1, 2024.

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
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CRYSTALLOGRAPHY IN THE NEWS

February 14, 2024
Researchers from France, Germany, Switzerland, the UK and the US report on the effects of multiphoton absorption on carbonmonoxy myoglobin in ultrafast pump-probe experiments.
February 15, 2024
Scientists from the US have synthesized and performed a ligand binding study on an antibiotic preorganized for ribosomal binding that overcomes antimicrobial resistance.
February 15, 2024
Researchers from the University of Liverpool observed superionic Li ion transport in $Li_7Si_2S_7$.

TIP OF THE MONTH

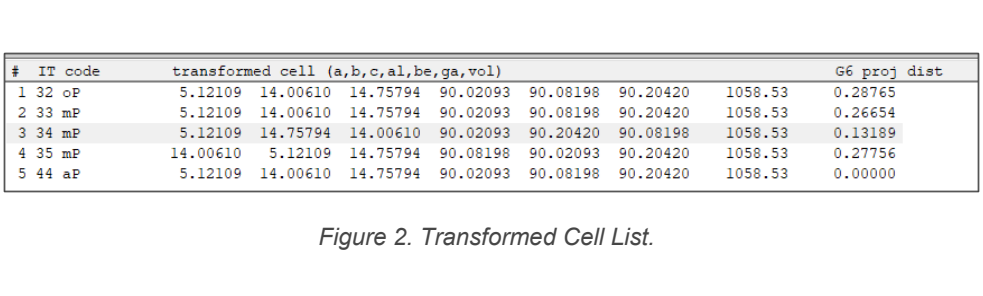
Forcing a user-defined lattice for processing

What is the issue?
CrysAlis^{Pro} may occasionally change the lattice upon processing and select the wrong one. This may occur even if the correct lattice was selected upon indexing. Let us hypothesize that this is taking place for a monoclinic unit cell with a beta angle close to 90° and CrysAlis^{Pro} has mistakenly set the lattice to orthorhombic.
How to select the correct monoclinic unit cell?
First and foremost, one must reindex the diffraction pattern in the correct monoclinic unit cell.

1. In **Lattice Wizard**, run **Peak hunting** and **Unit cell finding** as usual.
2. Click on the blue button 'Lattice transformation':

Figure 1. Lattice transformation button in Lattice Wizard.

3. Select the desired unit cell from the list displayed, as shown below, and click **OK**:



#	IT code	transformed cell (a,b,c,al,be,ga,vol)							G6 proj dist
1	32 oP	5.12109	14.00610	14.75794	90.02093	90.08198	90.20420	1058.53	0.28765
2	33 mP	5.12109	14.00610	14.75794	90.02093	90.08198	90.20420	1058.53	0.26654
3	34 mP	5.12109	14.75794	14.00610	90.02093	90.20420	90.08198	1058.53	0.13189
4	35 mP	14.00610	5.12109	14.75794	90.08198	90.02093	90.20420	1058.53	0.27756
5	44 aP	5.12109	14.00610	14.75794	90.02093	90.08198	90.20420	1058.53	0.00000

Figure 2. Transformed Cell List.

How to force a lattice type onto CrysAlis^{Pro}?

One must now set CrysAlis^{Pro} so it will not change the lattice type on its own.

4. Go back to **Lattice transformation** but this time, click on the small, blue arrow and select **Lattice transformation with user matrix**:

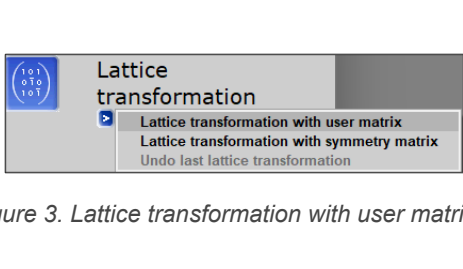


Figure 3. Lattice transformation with user matrix.

5. The line of 9 numbers displayed is in fact a 3 x 3 matrix that one can use to alter the unit cell dimensions. In this case, the dimensions are already correct from the previous indexing. So, just select **Apply:**

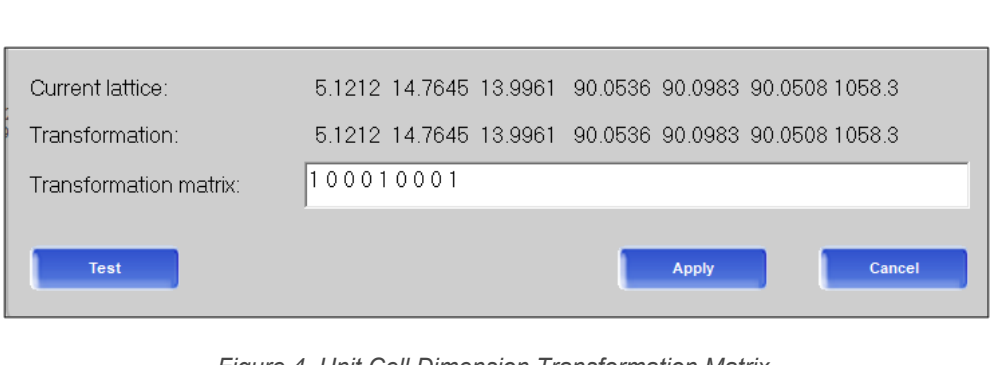


Figure 4. Unit Cell Dimension Transformation Matrix.

6.The primitive cell is displayed. Check the **User cell** box and select the desired lattice type and body centering option. Then, click **OK**:

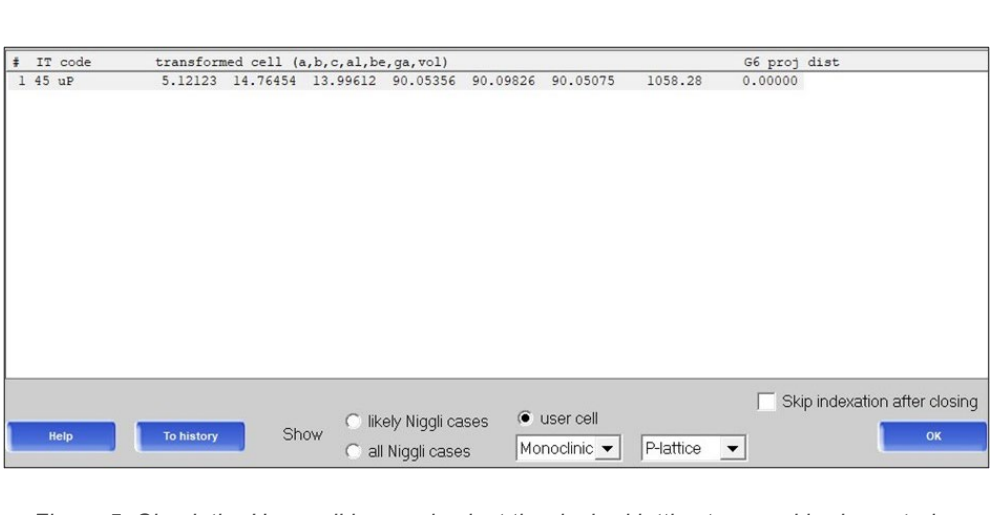


Figure 5. Check the User cell box and select the desired lattice type and body centering option.

7. The correct lattice is now displayed, and it is preceded by the code *UmP,* which signifies user-monoclinic-primitive:

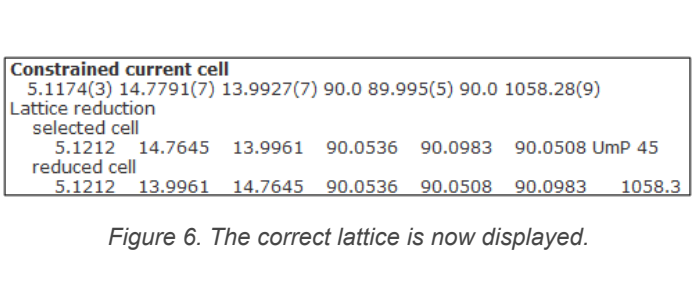
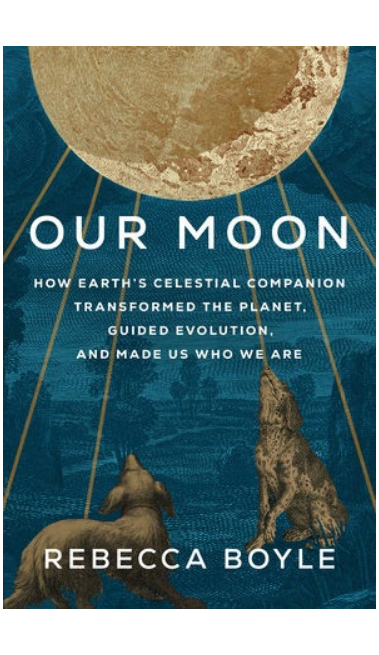


Figure 6. The correct lattice is now displayed.

8. Close **Lattice Wizard** and proceed with data processing. The user-defined cell and lattice will be kept by CrysAlis^{Pro} throughout data integration, scaling and space group search.

BOOK REVIEW



Review: *Our Moon: How Earth's Celestial Companion Transformed the Planet, Guided Evolution, and Made Us Who We Are*
By Rebecca Boyle
ISBN 9780593129722

Rebecca Boyle's *Our Moon: How Earth's Celestial Companion Transformed the Planet, Guided Evolution, and Made Us Who We Are* is an ambitious journey across time and space, documenting the history of Earth's Moon both as a physical object moving through the cosmos and as a metaphorical lens through which much of human history can be viewed.

Boyle begins with a historical anecdote from World War II, describing an incident where an Allied invasion of a Japanese island went awry—an event Boyle has a personal connection to, as her grandfather was one of the American soldiers there. The culprit was none other than the Moon. The tides didn't rise and the Allied forces were overexposed as they took the island. Boyle uses this event to set the stage, giving a real example laced with personal importance to indicate the vast range of impact something as seemingly simple as the Moon can have on human history—including her own.

Our Moon is divided into three parts. The first details our scientific understanding of the Moon—where it came from, how it was made, and when it was made. The second part details how the Moon played a role in human evolution and the evolution of human civilization. Early cultures not only worshiped the Moon but used it as a means of telling time beyond the singular day tracked by the rising and setting of the Sun. This allowed them to keep track of changes in the seasons, which was critical for the development of agricultural society. The third part details how our understanding of the Moon—and the race to set foot on it—has evolved since it was first viewed through a telescope. Boyle describes her own "visit to the Moon" —a trip to the Johnson Space Center in Houston, where a room full of Moon rocks is under strict lockdown behind a door designed for the Federal Reserve vaults, open only to a select few in special airtight suits dedicated to studying the Moon's unique geology.

Boyle's narrative style, though not strictly linear, is effortless to read, each sentence spun with spectacular grace and efficiency. It's easy to forget *Our Moon* is nonfiction because nonfiction works are often mostly focused on the conveyance of information, rather than well-crafted writing. *Our Moon* balances critical detail and concise description masterfully, making for prose so elegant it almost eclipses the subject matter.

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
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Register now >

UPCOMING EVENTS:

Pittcon 2024, February 24- 28, 2024, San Diego, CA

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.

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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

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