

Crystallography Newsletter  
Volume 11, No. 10, October 2019

[Subscribe](#)

## In this issue:

- [Crystallography in the News](#)
- [Visit with Us](#)
- [Join ROD on LinkedIn](#)
- [Product Spotlight](#)
- [Rigaku User Meeting](#)
- [Wizard Cryo](#)
- [Rigaku X-ray Forum](#)
- [Lab in the Spotlight](#)
- [Survey of the Month](#)
- [Last Month's Survey](#)
- [Useful Links](#)
- [Video of the Month](#)
- [Recent Crystallographic Papers](#)
- [Book Review](#)

## Visit with Us

[Southeastern Regional Meeting of the ACS](#)  
October 20-23, Savannah, Georgia

[Pittsburgh Diffraction Conference](#)  
October 24-26, Oak Ridge National Laboratory

[Protein Structure Determination in Industry](#)  
November 3-5, Hinxton, UK

[Southwest Regional Meeting - ACS](#)  
November 13-16, El Paso, Texas

[Asian Crystallographic Association 2019](#)  
December 17-20, Singapore

## Join ROD on LinkedIn

[Rigaku Oxford Diffraction 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.

## Rigaku User Meeting CrysAlis<sup>Pro</sup>/Olex<sup>2</sup> Workshop

March 24-26, 2020  
Rigaku Americas Corporation  
The Woodlands, TX



## Crystallography in the News

**October 1, 2019.** Zoë Fisher and Katarina Koruza from the ESS Deuteration and Macromolecular Crystallization (DEMAX) Support lab and Lund University have been using [vapor diffusion methods to grow large deuterated protein crystals](#) for neutron techniques as part of SINE2020's Crystal Growth work package.

**October 4, 2019.** Electron paramagnetic resonance ([EPR spectroscopy on protein single crystals](#)) is the ultimate method for determining the electronic structure of paramagnetic intermediates at the active site of an enzyme and relating the magnetic tensor to a molecular structure.

**October 7, 2019.** The [2019 Nobel Prize in Physiology or Medicine](#) has been awarded to National Institutes of Health grantees Gregg L. Semenza, M.D., Ph.D., of Johns Hopkins University, Baltimore, and William G. Kaelin Jr., M.D., of Dana-Farber Cancer Institute, Boston, who share the prize with Sir Peter J. Ratcliffe, M.D., of the University of Oxford, England, and Francis Crick Institute, London, for their discoveries of how cells sense and adapt to oxygen availability.

**October 9, 2019.** A new study by chemists at the University of Arkansas shows that X-ray crystallography can provide [inaccurate information about a critical set of proteins](#) - those found in cell membranes - which in turn could be leading to poor and inefficient drug design.

**October 9, 2019.** The [2019 Nobel Prize in Chemistry](#) has been awarded to John B. Goodenough (University of Texas at Austin), M. Stanley Whittingham (State University of New York at Binghamton), and Akira Yoshino (Meijo University) for their work on "the development of lithium ion batteries," according to the Nobel committee. "Lithium ion batteries have revolutionized our lives and are used in everything from mobile phones to laptops and electric vehicles," tweeted the committee. "Through their work, this year's Chemistry Laureates have laid the foundation of a wireless, fossil fuel-free society," it added. The three winners will share a prize of 9 million Swedish kroner (\$910,000).

**October 14, 2019.** A [new refrigeration technology based on the twisting and untwisting of fibres](#) has been demonstrated by a team led by Zunfeng Liu at Nankai University in China and Ray Baughman at the University of Texas at Dallas. As the demand for refrigeration expands worldwide, their work could lead to the development of new cooling systems that do not employ gases that are harmful to the environment.

**October 16, 2019.** If you travel to the outskirts of a town called Pulpí in Spain, you'll find an abandoned silver mine. Descend about 50 metres (164 feet) into it, and you'll enter a strange, shimmering room quite unlike anywhere else on Earth. Scientists might have finally found the [origin of this surreal jagged crystal cave](#).

**October 16, 2019.** Monash scientists have identified a survival mechanism of bacteria that cause disease in plant and animals, including highly virulent *E. coli* (*Escherichia coli*) related diseases. In a study published in *PLoS Genetics*, researchers show that [pathogenic bacteria obtain the essential nutrient iron during infection by pirating it](#) from host proteins.

**October 21, 2019.** Phagocytosis can be viewed as a primitive immune system used by all cells. When a pathogen is near the cell, the cell membrane will deform to engulf the pathogen and dispose of it. Researchers have found that a [two-dimensional sheet formed by the protein GAS7 is critical for this process](#), identifying through crystallography and microscopy two key hydrophilic loops in the protein.

## Product Spotlight

### [HyPix-6000HE: Hybrid photon counting X-ray detector](#)

Rigaku Oxford Diffraction now offers the [HyPix-6000HE Hybrid Photon Counting \(HPC\) X-ray detector](#). Like all HPCs, the HyPix-6000HE offers direct X-ray photon counting, single pixel point spread function and extremely low noise. The HyPix-6000HE HPC offers a small



We are pleased to announce that we will be holding a three-day user meeting and workshop at Rigaku Americas Corporation headquarters in The Woodlands, TX. The meeting will start Tuesday, March 24, 2020 and conclude Wednesday, March 25. The workshop will begin on March 25 and conclude March 26.

[Registration Form](#)

### Wizard Cryo formulations will flash-freeze to a clear amorphous glass in liquid nitrogen

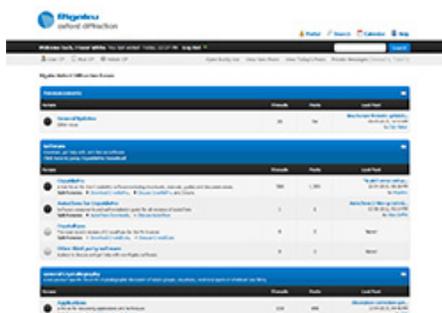


Rigaku Reagents' Wizard Cryo formulations will flash-freeze to a clear amorphous glass in liquid nitrogen or in the cryo-stream at 100K. There are eleven different cryocrystallants and sparing use of glycerol ensures a broad sampling of possible cryo conditions. Crystals can be frozen directly from their growth chambers, thus avoiding the additional step of pre-equilibration with an artificial cryo-solvent that can damage the crystal. These screens are offered in either a 96 deep well block plate format or in 10 ml tubes.

- 1009536: Wizard Cryo 1 Tubes \$325
- 1009537: Wizard Cryo 2 Tubes \$325
- 1009538: Wizard Cryo 1 & 2 Tubes \$600
- 1008649: Wizard Cryo 1 & 2 Block \$275

Contact [ReagentOrders@Rigaku.com](mailto:ReagentOrders@Rigaku.com)  
For more information, visit the [Rigaku Reagents website](#).

### Rigaku Oxford Diffraction Forum



pixel size of 100 microns, which allows you to better resolve reflections for long unit cells as well as improving reflection profile analysis. The HyPix-6000HE has a high frame rate of 100 Hz, as well as a unique Zero Dead Time mode providing the ultimate in error-free shutterless data collection.

Detector	HyPix-6000HE
Active area	77.5 mm x 80.0 mm
Dynamic quantum efficiency (Cu-Ka)	> 98%
Dynamic range	31-bits
Counting rate per pixel	1 x 10 <sup>6</sup> X-ray photons/sec
Readout speed	0 ms in ZeroDeadTime mode
Maximum frame rate	100 Hz
Point-spread function	1 pixel
Cooling	Air-cooled
Humidity control	Not required
Pixel size	100 µm x 100 µm



### Lab in the Spotlight

#### UCB Laboratory



The UCB Laboratory on Bainbridge Island is responsible for the majority of the crystallography work by the [Seattle Structural Genomics Center for Infectious Disease \(SSGCID\)](#). SSGCID is one of two Centers funded by NIAID in response to RFP-NIAID-DMID-NIHAI2016061, RFP-NIH-NIAID-DMID-07-19 and RFP-NIAID-DMID-NIHAI2011124 and is a consortium of four Pacific Northwest institutions (Seattle Children's Research Institute, University of Washington, UCB and Washington State University). SSGCID's primary mission is to determine the 3D atomic structures of proteins

and other molecules with an important biological role in human pathogens themselves, or molecules involved in host-pathogen interactions, by applying state-of-the art high-throughput (HTP) technologies and methodologies. Pathogens include those on the NIAID Category A-C agents as well as emerging and re-emerging infectious disease organisms, each year for a period of five years. This program supports research projects that utilize experimental approaches to better characterize the molecular mechanisms of protein targets and gain further insight into the functional roles of these targets. SSGCID at UCB is managed by co-PIs Tom Edwards and Peter Horanyi, site manager Don Lorimer. Jan Abendroth manages the x-ray data collection, structure solution and upkeep of the in-house system.

A quick survey of the PDB shows that in 12 years of SSGCID activity, the group has deposited 1209 structures. Of those 1209 structures, 314 were solved using data collected on the Rigaku home laboratory equipment at UCB. The equipment currently includes an FR-E+ Superbright outfitted with a pair of Osmic optics, AFC11 goniometers, Saturn 944+ CCD detectors and ACTOR sample changers. Below is a picture of the system. One very interesting note about the SSGCID's deposits is that over 50 were solved using iodine quick soaks. Even though the system is eleven (11) years old it is still used on a daily basis for the SSGCID's ongoing projects as well as UCB's internal projects.

### Useful Links

You may already have seen this posted on CNET, Apple News or Popular Mechanics; nevertheless, I am posting here this because it is so cool: [Miners find diamond trapped inside another diamond](#).

CrysAlis<sup>Pro</sup> V40 has been released on the Rigaku Oxford Diffraction Forum:

The major features of version 40 include:

- 32- and 64-bit versions
- Support of new AutoChem4.0 with an updated StructureExplorer
- Ewald3D live in the 64-bit version
- Extended support for multi-core use (in the 64-bit version, up to 32 cores)
- Significantly faster processing in dc profit
- Support of all new XtaLAB Synergy and ROD platforms
- Automated/manual version updating

### Survey of the Month

#### October 19 SCX Survey

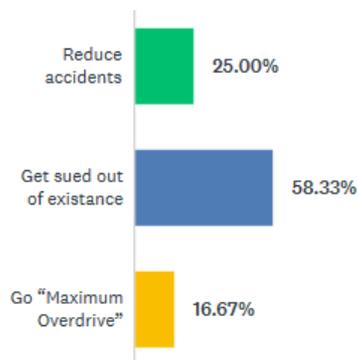
One way to be environmentally friendly is to read and maintain journals and periodicals in digital format. Of the work-related material you read, what percent is in digital format?

- <25%
- 25% to 50%
- 50% to 75%
- >75%

[Take the Survey](#)

### Last Month's Survey

Self-driving cars are almost here. They will:



### Video of the Month

This is not a video but nevertheless worthy of note. The link below takes you to a BBC Radio program on the life of Nobelist Dorothy Hodgkin,

## Selected Recent Crystallographic Papers

**Evolving SAXS versatility: solution X-ray scattering for macromolecular architecture, functional landscapes, and integrative structural biology.** Brosey, Chris A; Tainer, John A. *Current Opinion in Structural Biology*. Oct2019, Vol. 58, p197-213. 17p. DOI: [10.1016/j.sbi.2019.04.004](https://doi.org/10.1016/j.sbi.2019.04.004).

**From then till now: changing data collection methods in single crystal X-ray crystallography since 1912.** Powell, Harold R. *Crystallography Reviews*. Oct2019, Vol. 25 Issue 4, p264-294. 31p. DOI: [10.1080/0889311X.2019.1615483](https://doi.org/10.1080/0889311X.2019.1615483).

**An industry perspective of crystallography: its communities and its educational courses and labs.** Sišak Jung, Dubravka. *Crystallography Reviews*. Oct2019, Vol. 25 Issue 4, p295-315. 21p. DOI: [10.1080/0889311X.2019.1631295](https://doi.org/10.1080/0889311X.2019.1631295).

**Sequence and structure determination of a metalloproteinase: integration of mass spectrometry, phylogenetic and crystallography.** Borges, Rafael Junqueira; Marchi Salvador, Guilherme Henrique; Dos Santos, Lucilene Delazari; Uson, Isabel; De Mattos Fontes, Marcos Roberto. *Toxicon*. Oct2019:Supplement 1, Vol. 168, pS12-S12. 1p. DOI: [10.1016/j.toxicon.2019.06.066](https://doi.org/10.1016/j.toxicon.2019.06.066).

**3D printed droplet generation devices for serial femtosecond crystallography enabled by surface coating.** Echelmeier, Austin; Kim, Daihyun; Cruz Villarreal, Jorvani; Coe, Jesse; Quintana, Sebastian; Brehm, Gerrit; Egatz-Gomez, Ana; Nazari, Reza; Sierra, Raymond G.; Koglin, Jason E.; Batyuk, Alexander; Hunter, Mark S.; Boutet, Sébastien; Zatsopin, Nadia; Kirian, Richard A.; Grant, Thomas D.; Fromme, Petra; Ros, Alexandra. *Journal of Applied Crystallography*. Oct2019, Vol. 52 Issue 5, p997-1008. 12p. DOI: [10.1107/S1600576719010343](https://doi.org/10.1107/S1600576719010343).

**A prototype system for dynamically polarized neutron protein crystallography.** Pierce, J.; Crow, L.; Cuneo, M.; Edwards, M.; Herwig, K.W.; Jennings, A.; Jones, A.; Li, L.; Meilleur, F.; Myles, D.A.A.; Robertson, L.; Standaert, R.; Wonder, A.; Zhao, J.K. *Nuclear Instruments & Methods in Physics Research Section A*. Oct2019, Vol. 940, p430-434. 5p. DOI: [10.1016/j.nima.2019.06.023](https://doi.org/10.1016/j.nima.2019.06.023).

**Well-based crystallization of lipidic cubic phase microcrystals for serial X-ray crystallography experiments.** Andersson, Rebecka; Safari, Cecilia; Båth, Petra; Bosman, Robert; Shilova, Anastasya; Dahl, Peter; Ghosh, Swagatha; Dunge, Andreas; Kjeldsen-Jensen, Rasmus; Nan, Jie; Shoeman, Robert L.; Kloos, Marco; Doak, R. Bruce; Mueller, Uwe; Neutze, Richard; Brändén, Gisela. *Acta Crystallographica: Section D, Structural Biology*. Oct2019, Vol. 75 Issue 10, p937-946. 10p. DOI: [10.1107/S2059798319012695](https://doi.org/10.1107/S2059798319012695).

**Deriving and refining atomic models in crystallography and cryo-EM: the latest Phenix tools to facilitate structure analysis.** Klaholz, Bruno P. *Acta Crystallographica: Section D, Structural Biology*. Oct2019, Vol. 75 Issue 10, p878-881. 4p. DOI: [10.1107/S2059798319013391](https://doi.org/10.1107/S2059798319013391).

**Impact of the ΔPhe configuration on the Boc-Gly-ΔPhe-NHMe conformation: experiment and theory.** Buczek, Aneta; Siodlak, Dawid; Bujak, Maciej; Makowski, Maciej; Kupka, Teobald; Broda, Malgorzata A. *Structural Chemistry*. Oct2019, Vol. 30 Issue 5, p1685-1697. 13p. DOI: [10.1007/s11224-019-01387-w](https://doi.org/10.1007/s11224-019-01387-w).

**A new octa-Mn-substituted poly(polyoxotungstate).** Li, Hai-Lou; Lian, Chen; Yin, Da-Peng; Yang, Guo-Yu. *Dalton Transactions: An International Journal of Inorganic Chemistry*. 10/14/2019, Vol. 48 Issue 38, p14306-14311. 6p. DOI: [10.1039/c9dt02805f](https://doi.org/10.1039/c9dt02805f).

**New class of non-symmetrical homo-dibenzimidazolium salts and their dinuclear Silver(I) di-NHC complexes.** Haziz, Umie F.M.; Haque, Rosenani A.; Amirul, A.A.; Aidda, O.Noor; Razali, Mohd R. *Journal of Organometallic Chemistry*. Oct2019, Vol. 899, pN.PAG-N.PAG. 1p. DOI: [10.1016/j.jorganchem.2019.120914](https://doi.org/10.1016/j.jorganchem.2019.120914).

**Three dimensional manganese(II) coordination polymers constructed from 2,2-dimethylglutarate and bis(pyridyl) type ligands.** Köse Yaman, Pelin; Erer, Hakan; Yesilel, Okan Zafer. *Polyhedron*. Oct2019, Vol. 171, p317-322. 6p. DOI: [10.1016/j.poly.2019.07.008](https://doi.org/10.1016/j.poly.2019.07.008).

**Euphonoids A-G, cytotoxic diterpenoids from *Euphorbia fischeriana*.** Yan, Xue-Long; Zhang, Jun-Sheng; Huang, Jia-Luo; Zhang, Yao; Chen, Jia-Qi; Tang, Gui-Hua; Yin, Sheng. *Phytochemistry*. Oct2019, Vol. 166, pN.PAG-N.PAG. 1p. DOI: [10.1016/j.phytochem.2019.112064](https://doi.org/10.1016/j.phytochem.2019.112064).

**Understanding the structure and role of DNA-PK in NHEJ: How X-ray diffraction and cryo-EM contribute in complementary ways.** Wu, Qian; Liang, Shikang; Ochi, Takashi; Chirgadze, Dimitri Y.; Huiskonen, Juha T.; Blundell, Tom L. *Progress in*

hosted by Melvyn Bragg (yes, a relative of THE Braggs), in which he interviews Georgina Ferry, science writer and Hodgkin biographer, Judith Howard, Professor of Chemistry at Durham University, and Patricia Fara, Fellow of Clare College, Cambridge.



Watch the Video

Subscribe to Rigaku eNewsletters



Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on X-ray crystallography.

[www.Rigaku.com/en/subscribe](http://www.Rigaku.com/en/subscribe)

*Biophysics & Molecular Biology*. Oct2019, Vol. 147, p26-32. 7p. DOI: [10.1016/j.pbiomolbio.2019.03.007](https://doi.org/10.1016/j.pbiomolbio.2019.03.007).

**Discrete n-Stacks from Self-Assembled Perylenediimide Analogues.** Su, Feng; Chen, Guangmei; Korevaar, Peter A.; Pan, Fangfang; Liu, Huijiao; Guo, Zongxia; Schenning, Albertus P. H. J.; Zhang, Hui-Jun; Lin, Jianbin; Jiang, Yun-Bao. *Angewandte Chemie International Edition*. Oct2019, Vol. 58 Issue 43, p15273-15277. 5p. DOI: [10.1002/anie.201907838](https://doi.org/10.1002/anie.201907838).

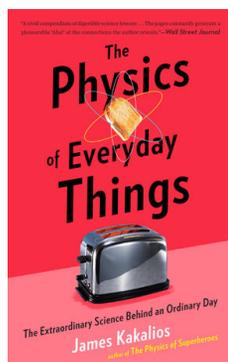
**A history and an industry perspective of crystallography.** Bombicz, Petra. *Crystallography Reviews*. Oct2019, Vol. 25 Issue 4, p263-263. 1p. DOI: [10.1080/0889311X.2019.1641098](https://doi.org/10.1080/0889311X.2019.1641098).

**Biological small angle scattering:** by Eaton E. Lattman, Thomas D. Grant and Edward H. Snell (IUCr Monographs on Crystallography 29, Oxford Science Publications), Oxford University Press, 2018, 268 pp., £65, ISBN 978-0-19-967087-1. By: Bóta, Attila. *Crystallography Reviews*. Oct2019, Vol. 25 Issue 4, p316-318. 3p. DOI: [10.1080/0889311X.2019.1592168](https://doi.org/10.1080/0889311X.2019.1592168).

## Book Review

*The Physics of Everyday Things: The Extraordinary Science Behind an Ordinary Day*

By James Kakalios  
ISBN 978-0-7704-3775-6



James Kakalios' newest book is a delightful endeavor into the physics of everyday life. Kakalios does not take the time to explain the basic concepts of physics, but rather the basic (or not-so-basic) physics of mundane mechanisms. These range from alarm clocks and toasters to car engines and airplanes—all things that we largely take for granted in our everyday lives. At times, Kakalios leans towards oversimplification of certain concepts, but as he himself admits in the chapter where he explains how an MRI machine works, "if you know all this—why are you reading this book?"

*The Physics of Everyday Things* is not geared towards physicists or engineers, but rather physics enthusiasts. The ideal audience for this book might be a younger student of physics—perhaps a high school student or college freshman—or someone who hasn't studied physics since their earlier

days. In order to enjoy the book and thoroughly appreciate it, the reader must have some knowledge of physics fundamentals. But someone who lives and breathes physics for a living might find it a little too trite to be entertaining.

*How To: Absurd Scientific Advice for Common Real-World Problems*

By Randall Munroe  
ISBN 978-0525537090



This is the latest work from the mind of Randall Munroe, best known for his hysterical online comic strip *xkcd*. If you are a fan of Munroe's comics, you will certainly enjoy this book. It combines his iconic comic style with very scientific pseudo self-help advice.

Mostly, Munroe takes real-world problems and scenarios and performs a reverse *reductio ad absurdum*, presenting the reader with the most absurd yet scientifically sound solutions to some terribly banal inquiries. Would they work in actuality? Possibly not, but they work in theory—and make for wildly entertaining hypothetical scenarios bolstered by delightfully sarcastic comic illustrations.

Some of the highlights include "How to Throw a Pool Party," "How to Move," "How to Play Tag," and "How to Build a Lava Moat." If you are thinking "one of these is not like the others," you are correct. "How to Build a Lava Moat" is an example of one of the chapters that answered a question I don't imagine most readers would have ever thought to ask, although the resulting response is highly entertaining. "How to Throw a Pool Party" was quite hilarious as well, as it operated under the initial assumption that one does not necessarily have a pool and needs to build one before hosting a party in it.

However, the best chapter was "How to Make an Emergency Landing." For this section, Munroe conducted a question-and-answer series with test pilot and astronaut Chris Hadfield. The contrast between Munroe's increasingly absurd queries, which include "How to Land on a Farm," "How to Land on an Aircraft Carrier," "How to Land on a Hostile Aircraft Carrier," and "How to Land a Space Shuttle in Downtown LA," and Hadfield's serious and scientifically sound expert responses, makes for a wildly entertaining departure from the typical format Munroe follows in his other chapters.

All in all, the book is a wonderfully comedic approach to everyday self-help grounded in very real but very absurd scientific solutions.

Reviews by Jeanette S. Ferrara, MA



**Rigaku Corporation**

e-mail: [info@Rigaku.com](mailto:info@Rigaku.com)  
Tel: +[81] 3-3479-0618  
FAX: +[81] 3-3479-6112

**Rigaku Americas**

e-mail: [info@Rigaku.com](mailto:info@Rigaku.com)  
Tel: (281) 362-2300  
FAX: (281) 364-3628

**Rigaku China**

e-mail: [info@Rigaku.com.cn](mailto:info@Rigaku.com.cn)  
Tel: +[86] 010-88575768  
FAX: +[86] 010-88575748

**Rigaku Europe**

e-mail: [info@Rigaku.com](mailto:info@Rigaku.com)  
Tel: +[49] 6102 77999 51  
FAX: +[49] 6102 77999 99

Copyright © 2019 — Rigaku Corporation and its Global Subsidiaries. All Rights Reserved

