

Crystallography Newsletter
Volume 10, No. 10, October 2018

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Come visit us at:

PSDI 2018: 26th Protein Structure Determination in Industry Meeting
Paris, France, November 11 – 13, 2018

AsCA 2018/CRYSTAL 32: Conference of the Asian Crystallographic Association (AsCA) and the Society of Crystallographers in Australia and New Zealand (SCANZ)
Auckland, New Zealand, December 2 – 5, 2018

2018 Jana Modulation Workshop
La Jolla, CA, USA, December 10 – 13, 2018

The CCDC is hiring

The CCDC is currently hiring for several positions throughout the organization. Specifically, they are searching for a User Support Scientist for their US Operation. This person will support the user community in North America by providing both technical and scientific support for a range of issues. They are looking for someone with knowledge of our software and familiarity with structural chemistry or drug discovery research.

For a detailed job description and person specification for the User Support Scientist and all open positions at CCDC, please see: <https://www.ccdc.cam.ac.uk/theccdcprofile/careers/>

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.

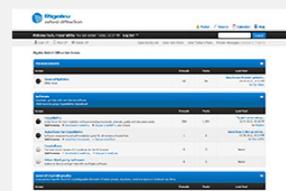
Rigaku Reagents: The Berkeley Screen



The Berkeley Screen was developed by researchers at the Lawrence Berkeley National Lab using statistical analyses of the Biological Macromolecular Crystallization Database. The screen has been extensively used to crystallize target proteins from the Joint BioEnergy Institute and the Collaborative Crystallography program at the Berkeley Center for Structural Biology. The screen contains 96 formulations as 1.7 mL volumes in a 96-well block plate.

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

Rigaku Oxford Diffraction Forum



www.Rigakuxrayforum.com

Here 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 CrystAlis^{PRO} software for single crystal data processing.

We look forward to seeing you on there soon.

Survey of the Month

October 18 SCX Survey

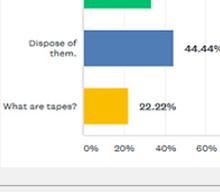
The Nobel Prize can be awarded to no more than three people for a given discovery or set of discoveries. Science has reached the point where discoveries are routinely being made by large teams of people working together over many years. Should scientists stop thinking of the Nobel Prize as the Holy Grail and think about other, more inclusive, prizes?

- Yes
- No

Take the Survey

Last Month's Survey

The other day I came across a box of 4 mm tape cartridges from the early 90s. I have no means to read them, other than perhaps through some expensive archive retrieval service. Any results from them have been long published.



Videos of the Month

Here is a very cool video showing the optical transforms of various objects – the last one is worth the wait.



Watch the Video

Here is a link to video describing how to make creamy ice cream safely with LN2:



Watch the Video

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Crystallography in the News

October 2, 2018. The connection between crystallography and quantum chemistry has always been very tight, after X-ray diffraction techniques became available in crystallography. The term **Quantum Crystallography** was first introduced in revisitation articles by L. Huang, L. Massa and Nobel Prize winner Jerome Karle, who associated it with two mainstreams: a) crystallographic information that enhances quantum mechanical calculations and b) quantum mechanical approaches to improve crystallography information.

October 3, 2018. MIT researchers have shown that some of the atoms in an enzyme called carbon monoxide dehydrogenase can rearrange themselves when oxygen levels are low. Catherine Drennan and her colleagues at MIT, Brandeis University, and Aix-Marseille University in France have now discovered a unique aspect of the **structure of the "C-cluster" – the collection of metal and sulfur atoms** that forms the heart of the enzyme carbon monoxide dehydrogenase (CODH). Instead of forming a rigid scaffold, as had been expected, the cluster can actually change its configuration.

October 9, 2018. To understand why some cancer cells resist radiotherapy, an international team of researchers has used **crystallography to "photograph" the first moments** of the molecular ballet that allows these cells to repair their DNA. The study involved teams from the CEA, CNRS, PROXIMA-1 beamline at SOLEIL, University of Paris-Sud, Gustave Roussy, Aix-Marseille University and University Paul Sabatier-Toulouse III.

October 9, 2018. **Thomas Steitz, who used X-ray crystallography** to determine the atomic structure of the ribosome, died of pancreatic cancer at age 78. Born in 1940, Steitz grew up in Wisconsin, where he studied chemistry at Lawrence College, graduating in 1962. He next went to Harvard University, and it was there, in 1963, that he first learned of X-ray crystallography. Dr. Steitz won the 2009 Nobel Prize in chemistry for his ribosome work.

October 12, 2018. On the basis of the rationale that the intra- and interparticle weak interactions play critical roles in growing high-quality single crystals of metal nanoparticles, an international group of scientists have **reproducibly obtained ideal crystals of Au₄₄(SR)₆₀** and successfully solved its structure by X-ray crystallography; this structure was theoretically predicted a decade ago and has long been pursued experimentally but without success until now.

October 14, 2018. Shekhar C. Mande, one of India's leading experts in DNA fingerprinting and diagnostics, was appointed **director-general of the Council of Scientific and Industrial Research (CSIR)**. He will head the 38 national research labs of CSIR located across the country, and also serve as secretary, Department of Scientific and Industrial Research. Mande was picked to replace biotechnologist Girish Sahni, who retired on 31 August.

October 15, 2018. The 48th Rosenstiel Award for Distinguished Work in Basic Medical Research has been awarded to **Professor Stephen C. Harrison** for his fundamental and far-reaching studies of protein structure using X-ray crystallography. Harrison is the Giovanni Armenise-Harvard Professor of Basic Medical Sciences and director of the Center for Molecular and Cellular Dynamics at the Harvard Medical School.

October 16, 2018. This month, the **U.S. Crystal Growing Competition** is marking its 5th year, and it's a glowing success. Over 250 teams have signed up this year, representing thousands of K-12 students and teachers, along with home-schooling families. Participants hail from 42 states and Washington D.C.

October 17, 2018. NASA Space Station On-Orbit Status. **BioServe Protein Crystallography (BPC)-1**: A crewmember used pipettes to mix varying viscosity solutions into the crystallization plates. BPC-1 seeks to demonstrate the feasibility of conducting protein crystal growth in real time onboard the ISS.

October 19, 2018. Cryo-electron microscopy (EM) can reveal small organic molecule structures with an **unprecedented combination of speed and certainty**, US scientists have shown. The team, based at University of California, Los Angeles (UCLA) and California Institute of Technology (Caltech) in Pasadena, obtained **molecular structures of 12 different compounds, each taking minutes. All were powders or amorphous solids** unsuitable for existing X-ray crystallography techniques.

October 19, 2018. Science's "Mother of Ribbon Diagrams" celebrates 50 years at Duke. **In 1981, Jane Richardson published her drawings for the first time** in the journal *Advances in Protein Chemistry*. Scientists immediately started using them and some even argued with her about how she'd depicted a particular molecule, opening up a new era of debate about scientific interpretation. In 1985, she was awarded a MacArthur Fellowship, the so-called "genius grant."

October 23, 2018. When chemists want to determine the structure of a molecule, they typically turn to X-ray crystallography. But chemists often find they can't grow the required large, high-quality crystals. Now, a similar technique, known as **electron crystallography**, which works with smaller crystals, is poised to become an alternative.

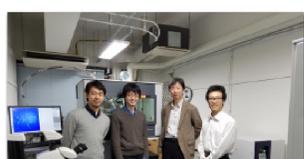
Product Spotlight



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 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.

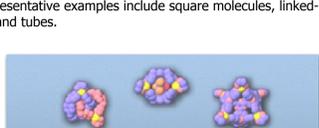
Detector	HyPix-6000HE
Active area	77.5 mm x 80.0 mm
Dynamic quantum efficiency (Cu-Kα)	> 98%
Dynamic range	31-bits
Counting rate per pixel	1 x 10 ⁶ X-ray photons/sec
Readout speed	0 ms in ZeroDeadTime mode
Maximum frame rate	100 Hz
Point-spread function	1 pixel
Cooling	Air-cooled
Humidity control	Not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

Lab in the Spotlight

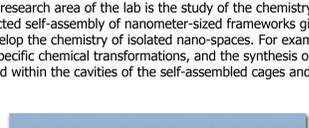


The Fujita Laboratory, Department of Applied Chemistry, The University of Tokyo

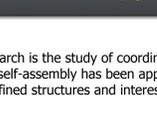
The Fujita lab studies three major topics in chemistry that are inspired by self-assembly in biological systems. First, self-assembling molecular systems utilizing transition metals. The simple combination of transition metal geometry with thoughtfully designed bridging ligands gives rise to the quantitative self-assembly of nanometer size, discrete organic frameworks. Representative examples include square molecules, linked-ring molecules, cages, capsules, and tubes.



The second major research area of the lab is the study of the chemistry of "isolated nano-space". Metal-directed self-assembly of nanometer-sized frameworks gives them an opportunity to develop the chemistry of isolated nano-spaces. For example, stabilization of labile molecules, specific chemical transformations, and the synthesis of labile molecules have been achieved within the cavities of the self-assembled cages and capsules.



The third and final area of research is the study of coordination polymers. In this study, the principle of metal-directed self-assembly has been applied to the preparation of non-covalent polymers with well-defined structures and interesting properties.



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Useful Link

What's ice cream, and why do we cream for it?
Summer is technically over but ice cream is a year-round treat. Here is an article about the science of ice cream from C&E News.

Selected Recent Crystallographic Papers

DynBench3D, a Web-Resource to Dynamically Generate Benchmark Sets of Large Heteromeric Protein Complexes. Bertoni, Martino; Aloy, Patrick. *Journal of Molecular Biology*. Oct2018, Vol. 430 Issue 21, p4431-4438. 8p. DOI: [10.1016/j.jmb.2018.09.011](https://doi.org/10.1016/j.jmb.2018.09.011).

PDFgetN3: a fast nuclear distribution functions from neutron diffraction data using ad hoc corrections. Juhás, Pavol; Louwen, Jaap N.; van Eijck, Lambert; Vogt, Eelco T. C.; Billinge, Simon J. L. *Journal of Applied Crystallography*. Oct2018, Vol. 51 Issue 5, p1492-1497. 5p. DOI: [10.1107/S1600576718010002](https://doi.org/10.1107/S1600576718010002).

Model-free classification of X-ray scattering signals applied to image segmentation. Lutz-Bueno, V.; Arboleda, C.; Leu, L.; Blunt, M. J.; Busch, A.; Georgiadis, A.; Bertier, P.; Schmatz, J.; Varga, Z.; Villanueva-Perez, P.; Wang, Z.; Lebugle, M.; David, C.; Stapanoni, M.; Diaz, A.; Guizar-Sicarios, M.; Menzel, A. *Journal of Applied Crystallography*. Oct2018, Vol. 51 Issue 5, p1378-1386. 8p. DOI: [10.1107/S1600576718011032](https://doi.org/10.1107/S1600576718011032).

A fast X-ray-diffraction-based method for the determination of crystal size distributions (FXD-CSD). Neher, Sigmund H.; Klein, Helmut; Kuhs, Werner F. *Journal of Applied Crystallography*. Oct2018, Vol. 51 Issue 5, p1352-1371. 19p. DOI: [10.1107/S1600576718010567](https://doi.org/10.1107/S1600576718010567).

Revised Crystal Structure of Human Adenovirus Reveals the Limits on Protein IX Quasi-Equivalence and on Analyzing Large Macromolecular Complexes. Kundhavai Natchiar, S.; Venkataraman, Sangita; Mullen, Tina-Marie; Nemerow, Glen R.; Reddy, Vijay S. *Journal of Molecular Biology*. Oct2018, Vol. 430 Issue 21, p4132-4141. 10p. DOI: [10.1016/j.jmb.2018.08.011](https://doi.org/10.1016/j.jmb.2018.08.011).

Structural Plasticity of Neurexin 1α: Implications for its Role as Synaptic Organizer. Liu, Jianfang; Misra, Anurag; Reddy, M.v.v.v. Sekhar; White, Mark Andrew; Ren, Gang; Rudenko, Gabby. *Journal of Molecular Biology*. Oct2018, Vol. 430 Issue 21, p4325-4343. 19p. DOI: [10.1016/j.jmb.2018.08.026](https://doi.org/10.1016/j.jmb.2018.08.026).

Fluoranthene and its n-extended diimides: Construction of new electron acceptors. Ishikawa, Hiroyuki; Katayama, Koji; Nishida, Jun-ichi; Kitamura, Chitoshi; Kawase, Takeshi. *Tetrahedron Letters: International Organ for the Rapid Publication of Preliminary Communications in Organic Chemistry*. Oct2018, Vol. 59 Issue 42, p3782-3786. 5p. DOI: [10.1016/j.tetlet.2018.09.012](https://doi.org/10.1016/j.tetlet.2018.09.012).

A Six-Crossing Doubly Interlocked [2]Catenane with Twisted Rings, and a Molecular Gantry Knot. Danon, Jonathan J.; Leigh, David A.; Pisanò, Simone; Valero, Alberto; Vitorica-yrezabal, Iñigo J. *Angewandte Chemie International Edition*. Oct2018, Vol. 57 Issue 42, p13833-13837. 5p. DOI: [10.1002/anie.201807135](https://doi.org/10.1002/anie.201807135).

Rational protein design for thermostabilization of glycoside hydrolases based on structural analysis. Watanabe, Masahiro; Matsuzawa, Tomohiko; Yaoi, Katsuro. *Applied Microbiology & Biotechnology*. Oct2018, Vol. 102 Issue 20, p8677-8684. 8p. DOI: [10.1007/s00253-018-9288-7](https://doi.org/10.1007/s00253-018-9288-7).

Rationally Designed Semisynthetic Natural Product Analogues for Stabilization of 14-3-3 Protein-Protein Interactions. Andrei, Sebastian A.; de Vink, Pim; Sijbesma, Eline; Han, Ling; Brunsfeld, Luc; Kato, Nobuo; Ottmann, Christian; Higuchi, Yusuke. *Angewandte Chemie*. 10/8/2018, Vol. 130 Issue 41, p13658-13662. 5p. DOI: [10.1002/ange.201806584](https://doi.org/10.1002/ange.201806584).

Crystal structure of mutant carboxypeptidase B from *Thermoactinomyces vulgaris* with an implanted S1' subsite from pancreatic carboxypeptidase B. Akparov, Valery Kh.; Timofeev, Vladimir I.; Kuranova, Inna P.; Raktitina, Tatiana V. *Acta Crystallographica: Section F: Structural Biology Communications*. Oct2018, Vol. 74 Issue 10, p638-643. 5p. DOI: [10.1107/S2053230X18011962](https://doi.org/10.1107/S2053230X18011962).

Architecture of the RNA polymerase II elongation complex: new insights into Sp4/5 and Elf1. Ehara, Haruhiko; Sekine, Jun-ichi. *Transcription (2154-1264)*. 2018, Vol. 9 Issue 5, p286-291. 6p. DOI: [10.1080/21541264.2018.1454817](https://doi.org/10.1080/21541264.2018.1454817).

Gene cloning, expression, and X-ray crystallographic analysis of a β-mannanase from *Eisenia fetida*. Ueda, Mitsuhiko; Hirano, Yu; Fukuhara, Hiroaki; Naka, Yuki; Nakazawa, Masami; Sakamoto, Tatsuji; Ogata, Yoshiyuki; Tamada, Taro. *Enzyme & Microbial Technology*. Oct2018, Vol. 117, p15-22. 8p. DOI: [10.1016/j.enzmictec.2018.05.014](https://doi.org/10.1016/j.enzmictec.2018.05.014).

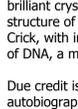
Resolving the Discrepancies Between Empirical and Rayleigh Charge Limiting Models for Globular Proteins. De Freitas, Karen C. B. *Journal of the American Society for Mass Spectrometry*. Oct2018, Vol. 29 Issue 10, p2059-2066. 8p. DOI: [10.1007/s13361-018-2025-8](https://doi.org/10.1007/s13361-018-2025-8).

Conformational response to charge clustering in synthetic intrinsically disordered proteins. Tedeschi, Giulia; Santambrogio, Carlo; Grandori, Rita; Brocchia, Stefania; Sallandini, Edoardo; Longhi, Silvia. *BBA - General Subjects*. Oct2018, Vol. 1862 Issue 10, p2204-2214. 11p. DOI: [10.1016/j.bbagen.2018.07.011](https://doi.org/10.1016/j.bbagen.2018.07.011).

Blind prediction of protein B-factor and flexibility. Bramer, David; Wei, Guo-Wai. *Journal of Chemical Physics*. 10/5/2018, Vol. 149 Issue 13, pN.PAG-N.PAG. 13p. 1 Diagram, 10 Charts, 4 Graphs. DOI: [10.1063/1.5048469](https://doi.org/10.1063/1.5048469).

Crystal structure of the major squasch formed in the sprangler, Stephen of the human c-MYC oncogene. Stump, Sascha; Mou, Tung-Chung; Sprang, Stephen R.; Natale, Nicholas R.; Beall, Howard D. *PLoS ONE*. 10/12/2018, Vol. 13 Issue 10, p1-15. 15p. DOI: [10.1371/journal.pone.0205584](https://doi.org/10.1371/journal.pone.0205584).

Book Review



The Equations of Life: How Physics Shapes Evolution
By Charles S. Cockell

Charles S. Cockell's *The Equations of Life* does a phenomenal job of presenting evolution from a new perspective. Cockell, an astrobiologist at the University of Edinburgh, states in the short preface, "This book explores one line of thinking that tries to make sense of diverse areas of science that straddle the living and the nonliving, the infeasible links between physics and evolutionary biology." *The Equations of Life* does just that, and does it quite well.

Without getting overly bogged down in minutiae, Cockell explores the building blocks of life on Earth—DNA, water, and carbon, to name a few of the better known ones—and details how they work on a physical level. For example, he explicates why having two hydrogens and an oxygen in a water molecule actually matters in terms of evolution and life on Earth. At the conclusion of the book, Cockell briefly extrapolates how life might or might not evolve on other planets, based on how it has evolved here and why it has evolved that way and not another.

Perhaps one of the best and most illustrative investigations involves the lesser mole-rat, *Nannopalax leucodon*. The first page of the book immediately following the table of contents features a black and white photograph of this creature, with the caption *P = F/A*. You might recognize this from a high school physics class, or even a middle school one: pressure equals force divided by area. But what does this have to do with the lesser mole-rat, you might ask? You'll have to read Cockell's book to find out—I don't want to spoil it for you.

One minor refreshing detail in Cockell's chapter on DNA involves Rosalind Franklin, a brilliant crystallographer whose work helped Watson and Crick model the molecular structure of DNA. Cockell gives credit where it is due: "When James Watson and Francis Crick, with inspiration from X-ray images made by Rosalind Franklin, proposed a structure of DNA, a monumental step forward was made in deducing the centerpiece of life."

Due credit is something Franklin was denied in her own time and in Watson's autobiographical retelling of history, *The Double Helix*. Even though Brenda Maddox's *Rosalind Franklin: The Dark Lady of DNA* came out 15 years ago, and Franklin's contributions to the discovery of DNA have been made better known in the years since her death, some authors still neglect to mention her when the subject of DNA is as it pertains to Watson and Crick surfaces in their work. So, it's always a refreshing and positive moment when an author like Cockell gives Franklin her due.

Despite its seemingly complex subject matter, *The Equations of Life* feels like a highly informative beach read in the best possible way. I could not put it down—Cockell's prose is engaging and fun—a perfect introduction to the fundamental connections between physics and evolutionary biology.

Review by Jeannette S. Ferrara, MA