Crystallography Times

Rigaku oxford diffraction

Crystallography Newsletter
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In this issue:

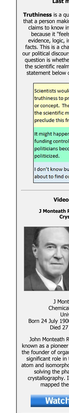
Rigaku Oxford Diffraction invites all users of Rigaku equipment to join us on our X-ray forum

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 Crysalis™ software for single crystal data processing.

We look forward to seeing you on there soon.

Survey of the month



Last month's survey

Truthiness is a quality characterizing a "truth" that a person making an argument or assertion claims to know intuitively "from the gut" or because it "feels right" without regard to evidence, logic, intellectual examination, or facts. This is a characteristic that has invaded our political discourse around the world, but the question is whether truthiness will also invade the scientific realm. Based on this, with what statement below do you most closely agree?

Scientists would never stoop to truthiness to promote an idea or concept. The very nature of the scientific method will preclude this from happening.	66.07%
It might happen if scientific funding controlled by politicians becomes politicized.	22.22%
I don't know but I guess we are about to find out.	11.11%

Video of the month

J Monteath Robertson – Chemical Crystallographer

J Monteath Robertson
Chemical Crystallographer
Univ of Glasgow
Born 24 July 1900, Auchterarder, Scotland.
Died 27 December 1989.

John Monteath Robertson ("JM") was best known as a pioneer of X-ray crystallography and the founder of organic crystallography, playing a significant role in the development of heavy-atom and isomorphous-replacement methods for solving the phase problem in chemical crystallography. In 1960 his research group mapped the structure of limonin.

Watch the Video

Upcoming events

Pittcon 2017, March 5 – 9, 2017 in Chicago, Illinois, USA

APS March Meeting, March 13 – 17, 2017 in New Orleans, LA, USA

2017 West Coast Protein Crystallography Workshop, March 19 – 22, 2017 in Pacific Grove, CA, USA

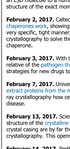
See full list >

Honey, I shrunk the crystallographers!

Peter Williams/Flickr

Strange Life Has Been Found Trapped Inside These Giant Cave Crystals >

ISBC Granada 2017



The Laboratorio de Estudios Cristalográficos announces the sixth International School on Biological Crystallization, to be held in Granada from May 29th to June 2nd, 2017.

This International School will focus on the fundamentals of crystallization and its application to biotechnology and to the life sciences.

ISBC2017 will provide five days of lectures and practical demonstrations related to the crystallization of biological macromolecules, biominerals and biomimetic materials, with one full day devoted to basic studies in the crystallization of membrane proteins, viruses and large macromolecular complexes.

For more about ISBC Granada 2017

Crystallography in the news

February 1, 2016. A new insight into how viruses replicate based on X-ray crystallography work by a team at Thomas Jefferson University could ultimately lead to new antiviral drugs to treat respiratory RNA viruses.

February 1, 2017. Researchers at the University of North Carolina School of Medicine, led by Daniel Anderson, Ph.D., and Sheng Wang, Ph.D., discovered that the LSD-to-receptor relationship functions much like a trash bin. The years-long experiment involved binding an LSD molecule to a human serotonin receptor, then producing the first-ever crystal structure of the exact moment they joined.

February 2, 2017. Caltech researchers are learning more about how ribosome chaperones work, showing that the above particular chaperone binds to its protein client in a very specific, tight manner, almost like a glove fitting a hand. The researchers used X-ray crystallography to decode the atomic structure of the ribosomal protein bound to its chaperone.

February 2, 2017. With the first detailed analysis of a cellular component from a close relative of the pathogen that causes tuberculosis, Rockefeller scientists are suggesting strategies for new drugs to curb this growing health problem.

February 13, 2017. Scientists have discovered a better way to extract proteins from the membranes that encase them, making it easier to study with X-ray crystallography how cells communicate with each other to create human health and disease.

February 13, 2017. Scientists have used high-intensity X-ray pulses to determine the structure of the crystalline protein envelope of an insect virus. The tiny viruses with their crystal casing are by far the smallest protein crystals ever analyzed using X-ray crystallography. This opens up new opportunities in the study of protein structures.

February 14, 2017. Perth researchers have uncovered a potential way to combat antibiotic-resistant superbugs that kill over 700,000 deaths a year globally. They have discovered a protein that causes multi-drug resistance by masking bacteria against the body's immune system and key types of antibiotics.

February 23, 2017. When Meytal Landau, a structural biologist at Technion???Israel Institute of Technology, recently solved the structure of some peptide fibrils she believed were amyloids, she nearly fell over her chair. She expected to see the ??-sheet architecture that???s common to all known amyloid fibrils. Instead, she saw the first known α-helical version.

February 23, 2017. Sexual reproduction and viral infections both rely on a functionally identical protein, according to research from the University of Maryland. The protein enables the fusion of two cells, such as sperm cell and egg cell, or the fusion of a virus with a cell membrane. The discovery suggests that the protein evolved early in the history of life on Earth, and new cross-kingdom opportunities in the study of protein fusion could help fight parasite infections.

February 24, 2017. Mike Sutton tells the tale of Nobel Prize winner John Kendrew, born 100 years ago this month, and his work towards the unveiling of protein structures.

Product spotlight: XtaLAB Synergy-S

One of the first customers of XtaLAB Synergy-S has characterized it by saying it's "like running your lab on steroids."

Using a combination of leading-edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S produces fast, precise data in an intelligent fashion.

The system is based around our NEW PhotonJet-S series of microfocus sources. These third generation sources have been designed to maximize X-ray photons at the sample by using a combination of new optics, new longer-life tubes and an improved alignment system.

The new Kappa goniometer has been completely redesigned to incorporate faster motor speeds and a unique telescopic two-theta arm to provide total flexibility for your diffraction experiment.

For more about XtaLAB Synergy-S

Lab in the spotlight

Professor Richard Cooper
Head of Chemical Crystallography
Associate Professor of Chemistry
Oxford University

The Chemical Crystallography Group and X-ray Crystallography Facility are located in the Chemistry Research Laboratory, Mansfield Road, Oxford. X-ray crystallography was established in Oxford in 1929 and has been part of the Department of Chemistry since 1946.

In addition to world-class X-ray diffraction facilities, Chem. Crystallography has an active research group and is home to the CRYSTALS software project. The group actively develops new experimental and computational methods in X-ray and neutron diffraction. Their research into the propensity of molecules to form crystals uses a set of chemiinformatics descriptors more commonly used in the field of drug discovery and applies them to a materials chemistry problem.

The Chemical Crystallography group has a long and prestigious history within the global crystallographic community and continues today to advance the boundaries of the field.

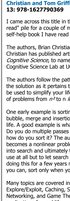
Useful link

Olex²: an immensely powerful crystallography program

Olex² handles very complex crystallographic tasks through an intuitive GUI. The graphical user interface is the result of 10 years of striving to provide the best possible experience to modelling even the most challenging structures with ease.

The software originated at Durham University and has been in active development since 2004. Currently in development are extensions to improve productivity, some of which are already available to try out.

Olex² is open source and therefore free software. However, the authors ask that you register on their website in order to download their software products so that they can provide update notifications, offer support, and also gain feedback about its usage and improve the software for everyone.



For instant access to their software and support services.

Selected recent crystallographic papers

Generalizing crystallography: a tribute to Alan L. Mackay at 90. Hargittai, I., *Struct Chem* (2017) 28, 1. DOI:10.1007/s11224-016-0768-1

Using X-Ray Crystallography to Simplify and Accelerate Biologics Drug Development. Mark L. Brader, *et al. Journal of Pharmaceutical Sciences*. Vol. 106, Issue 2, Feb 2017, Pages 477?494. DOI: 10.1016/j.xphs.2016.10.017

Room temperature neutron crystallography of drug resistant HIV-1 protease uncovers limitations of X-ray structural analysis at 100K. Oksana O. Gerlits, David A. Keen, Matthew P. Blakeley, John R.G. Kovalevsky, Irene T. Weber, and Andrey Y. Kovalevsky. *J. Med. Chem.*, Just Accepted Manuscript. DOI: 10.1021/acs.jmedchem.6b01767.

Isolation of a chiral anthracene cation radical: X-ray crystallography and computational interrogation of its racemization. Moon Y. Ivanov, Khadiza Thakur, Anshul Bhatnagarb and Rajendra Rathore. *Chem. Commun.*, 2017, Advance Article. DOI: 10.1039/C6CC09370C

The dramatic development of X-ray photocrystallography over the past six decades. Philip Coppens. *Structural Dynamics* 4, 032102 (2017); DOI: 10.1063/1.4975301.

Mapping-Out Catalytic Processes in a Metal???Organic Framework with Single-Crystal X-ray Crystallography. Sumby, Christopher J., Doonan, Christian J., et al. *Angewandte Chemie*. (2017) DOI: 10.1002/ange.201611254.

The first C(O)NH(PO)-based phosphonic triamide structure with an N···n → hydrogen bonding: a combination of X-ray crystallography and theoretical study to evaluate the strength of hydrogen bonds. Mahrizal Pourayoubi, et al. *Phosphorus, Sulfur, and Silicon and the Related Elements*. Accepted author version posted online: 21 Feb 2017. DOI: 10.1080/10426507.2017.1295360.

Crystal structure prediction guided by small-molecule single-crystal crystallography with crystal morphology prediction and molecular modelling. McArdle, Patrick. *Journal of Applied Crystallography*. Feb2017, Vol. 250 Issue 1, p1020-1026. 6p. DOI: 10.1107/S1600576716018466.

Structural Chemistry: The Last 50 Years as Seen by an X-ray Crystallographer. Burgi, Hans-Beat. *Journal of Chemistry*. Feb2017, Vol. 57 Issue 1, p109-116. 8p. DOI: 10.1002/jch.201600050.

Crystal structure of dicesium hydrogen citrate from laboratory single-crystal and powder X-ray diffraction data and DFT comparison. Rammohan, Alagappa; Sanjeeva, Amy A.; Kaduk, James A. *Acta Crystallographica: Section E* Feb2017, Vol. 73 Issue 2, p263-274. 12p. DOI: 10.1107/S2056989016020752.

Single crystal structure elucidation and thermoelectric properties of a long-periodically ordered germanium arsenic telluride. Nenning, Markus; Fahrnbauer, Felix; Kasprick, Marcus; Oeckler, Oliver. *Journal of Alloys & Compounds* Feb2017, Vol. 694, p1160-1164. 5p. DOI: 10.1016/j.jallcom.2016.10.104.

Robust Multifunctional Yttrium-Based Metal-Organic Frameworks with Breathing Effect. Firmino, Ana D. G.; Mendes, Ricardo F.; Antunes, Marijanda M.; Barbosa, Paula C.; Vilela, Sérgio M. F.; Figueiredo, Filipe M.; Figueiredo, Filipe M.; Tomé, João P. C.; Paz, Filipe A. Almeida. *Inorganic Chemistry* 2/6/2017, Vol. 56 Issue 3, p1330-1348. 19p. DOI: 10.1021/acs.inorgchem.6b02199.

Crystallometric and projective properties of Kikuchi diffraction patterns. Nolze, Gert; Winkelmann, Aimo. *Journal of Applied Crystallography* Feb2017, Vol. 250 Issue 1, p102-119. 17p. DOI: 10.1107/S1600576716017477.

Discovery of ambiguity in the traditional definitions of angle of diffraction and glancing angle. Bhattacharjee, Pramode Ranjan. *Optik - International Journal for Light & Electron Optics* Feb2017, Vol. 130, p702-707. 6p. DOI: 10.1016/j.ijleo.2016.10.114.

X-Ray Crystallographic Analysis, EPR Studies, and Computational Calculations of a Cu(II) Tetrameric Acid Complex. Matsadis, Dimitrios; Tanoos, Dimitrios; Stefanou, Valentina; Ypgless???Markopoulou, Olga; Mckee, Vickie; Sanakis, Yiannis; Lazarou, Katerina N.; Christopoulos, Athanasios; Yannopoulos, Spyros N.; Markopoulos, John H. *Bioinorganic Chemistry & Applications*. 2/19/2017, p1-10. 10p. DOI: 10.1155/2017/7950923.

Structural Chemistry, Fuzzy Logic, and the Law. Bernstein, Joel. *Israel Journal of Chemistry*. Feb2017, Vol. 57 Issue 2, p124-136. 13p. DOI: 10.1002/ijch.201600059.

Engineering Molecular Topology: A Pseudopeptidic Macrocyclic Figure-Eight Motif. Sharma, Sakshi; Thorat, Shridhar H.; Gonnade, Rajesh G.; Jasinski, Jerry P.; Butcher, Ray. *European Journal of Organic Chemistry* Feb2017, Vol. 2017 Issue 7, p1120-1124. 5p. DOI: 10.1002/ejoc.201601365.

Synthesis, chemo-enzymatic conjugation and click application to the X-ray structural determination of carbohydrate-lectin complexes using single/multi-wavelength anomalous dispersion phasing. Shimadzutsuru, Junpei; Maruta, Hisayoshi; Suzuki, Tatsuya; Nishikawa, Tosuke; Kawasaki, Masato; Imamura, Akihiro; Ishida, Hideharu; Ando, Hiromune; Kato, Ryuichi; Kiso, Makoto. *Bioorganic & Medicinal Chemistry*. Feb2017, Vol. 25 Issue 3, p1132-1142. 11p. DOI: 10.1016/j.bmc.2016.12.021.

***XLabPDF*, a program to obtain quantitative pair distribution functions from electron diffraction data.** Tran, Dung Trung; Svensson, Gunnar; Tai, Cheuk-Wai. *Journal of Applied Crystallography*. Feb2017, Vol. 250 Issue 1, p304-312. 8p. DOI: 10.1107/S1600576716019744.

Whaddaya Know: A Guide to Uncertainty and Subjectivity in Structural Biology. Mackay, Joel P.; Landsberg, Michael J.; Whitten, Andrew E.; Bond, Charles S. *Trends in Biochemical Sciences*. Feb2017, Vol. 42 Issue 2, p155-167. 13p. DOI: 10.1016/j.tibs.2016.11.002.

Book review

Algorithms to Live By: The Computer Science of Human Decisions By Brian Christian and Tom Griffiths, Henry Holt and Co, New York, 2016, 368 pp., ISBN-13: 978-1627790369

I came across this title in the list of books Amazon thought I might like. It sat in my "to read" pile for a couple of months until I finally read it over the holidays. It is the most fun self-help book I have read in quite a while.

The authors, Brian Christian and Tom Griffiths, are both experts in cognitive science. Christian has published articles in the *British Journal, The Atlantic, Wired*, and *Cognitive Science*; to name a few. Griffiths is the director of the Computational Cognitive Science Lab at Berkeley.

The authors follow the pattern of describing a problem in computer science, explaining the solution to a problem in computer science, then expounding upon how that solution can be used to simplify your life. The underlying theme is to reduce your effort on a number of problems from n² to n log n or slightly better.

One early example is sorting. The authors describe how various algorithms, like the bubble, merge and insertion sort, work and how to apply those algorithms to everyday life. A good example is what to do with the stack of email that greets you every morning. Do you do multiple passes on your inbox and prioritize? Do you sort email? If you sort, how do you sort it? The authors' solution to dealing with email is to go through it once or it becomes a nonlinear problem adding unnecessary work. The subject of sorting segues into caching algorithms and how computer scientists have developed ways to make efficient use of all but its last memory location. I find them for you when you need them. I've been doing this for a few years now, and it is a huge time saver. The lesson is: search when you can, sort only when you must, and don't sort if you don't search.

Many topics are covered in addition to sorting and searching: Optimal Stopping, Explore/Exploit, Caching, Scheduling, Bayes' Rule, Overfitting, Relaxation, Randomness, Networking, and Game Theory. Each topic is approached with examples of practical applications for real life.

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