Crystallography Times

Rigaku oxford diffraction

Crystallography Newsletter
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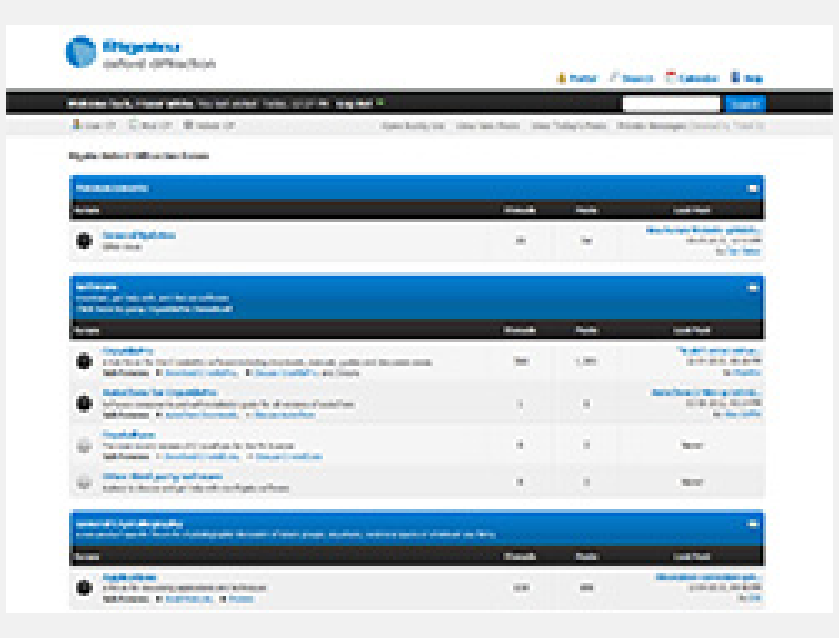
In this issue:

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

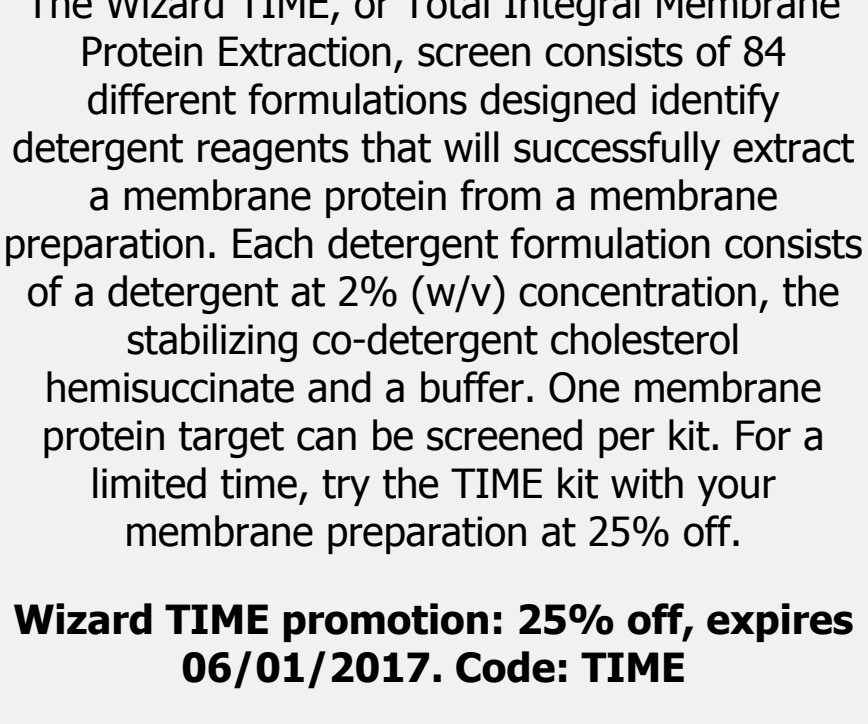


www.rigakuxrayforum.com

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^Pro software for single crystal data processing.

We look forward to seeing you on there soon.

Rigaku Reagents: Wizard TIME - 96-well block plate

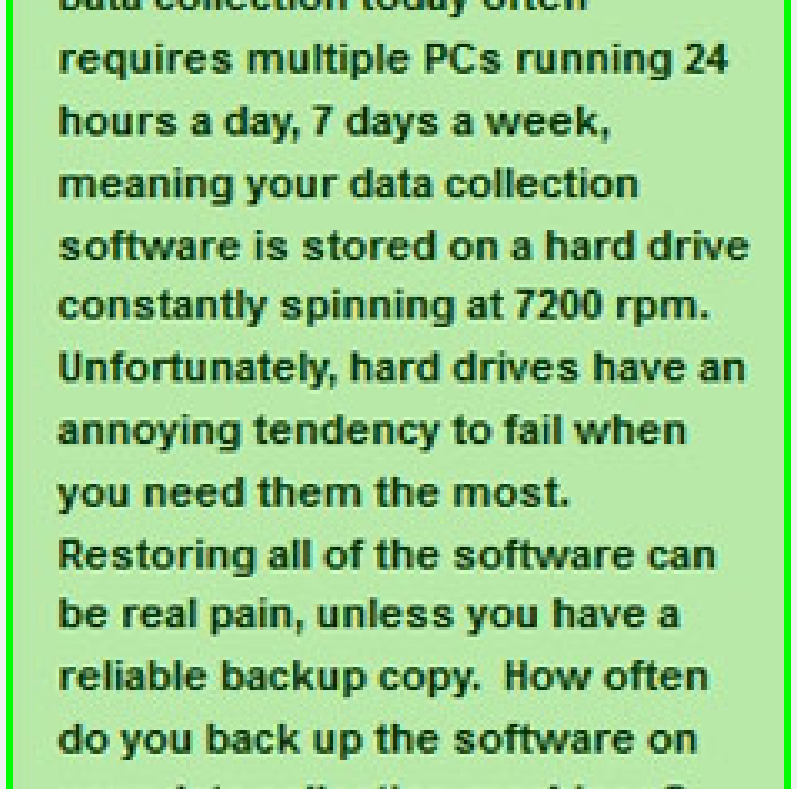


Membrane proteins require detergent solubilization for purification and crystallization. The Wizard TIME, or Total Integral Membrane Protein Extraction, screen consists of 84 different formulations designed identify detergent reagents that will successfully extract a membrane protein from a membrane preparation. Each detergent formulation consists of a detergent at 2% (w/v) concentration, the stabilizing co-detergent cholesterol hemisuccinate and a buffer. One membrane protein target can be screened per kit. For a limited time, try the TIME kit with your membrane preparation at 25% off.

Wizard TIME promotion: 25% off, expires 06/01/2017. Code: TIME

Contact ReagentOrders@Rigaku.com
For more information, visit the Rigaku Reagents website.

Survey of the month



Data collection today often requires multiple PCs running 24 hours a day, 7 days a week, meaning your data collection software is stored on a hard drive constantly spinning at 7200 rpm. Unfortunately, hard drives have an annoying tendency to fail when you need them the most. Restoring all of the software can be real pain, unless you have a reliable backup copy. How often do you back up the software on your data collection machines?

- Continuously.
- Once a month.
- Once a year, whether it needs it or not.
- Backups? We don't need no stinkin' backups.

Take the Survey

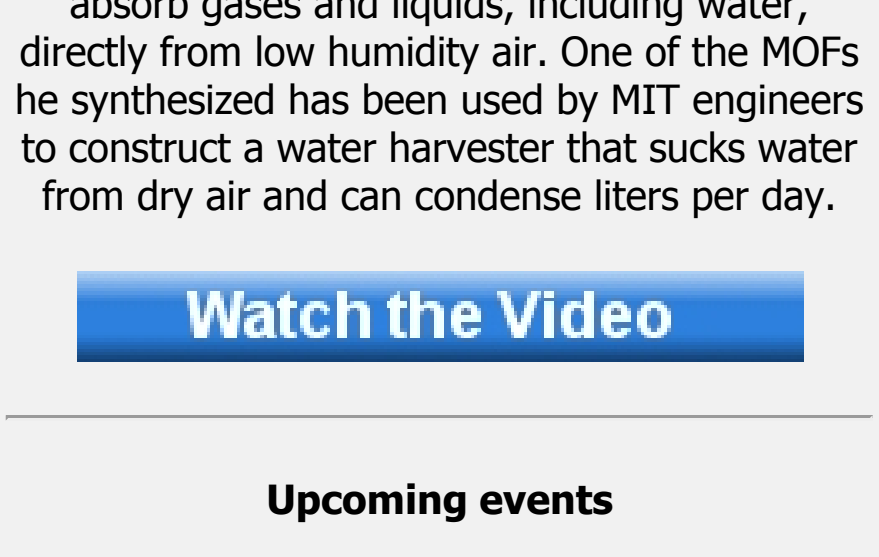
Last month's survey

It used to be almost essential for a crystallographer to know how to program so that special cases could be dealt with as they popped up in a research project. Now that everyone expects to be able to download an app onto a cell phone, how important is the knowledge of programming to effectively do crystallographic research?

There is plenty of good, free software available and the need to perform custom programming has all but disappeared.	35.71%
I would probably still be programming if FORTRAN was still popular but don't have the time to learn modern programming languages.	14.29%
A skill in programming is still an important part of being able to deal with special problems that crop up in crystallographic research.	35.71%
If I wanted to write code, I would go to work for Microsoft.	14.29%

Video of the month

Device pulls water from dry air, powered only by the sun



Metal-organic framework sucks up water from air with humidity as low as 20 percent

Omar Yaghi, a professor of chemistry at UC Berkeley, explains how metal-organic frameworks are built and how they are able to absorb gases and liquids, including water, directly from low humidity air. One of the MOFs he synthesized has been used by MIT engineers to construct a water harvester that sucks water from dry air and can condense liters per day.

Watch the Video

Upcoming events

MRS Spring Meeting & Exhibit, April 17 – 21, 2017 in Phoenix, Arizona, USA

Korea Lab, April 18 – 21, 2017 in Islan, Korea

62nd ISA Analysis Division Symposium, April 23 – 27, 2017 in Pasadena, CA, USA

See full list >

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Join ROD on LinkedIn

The 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.

Crystallography in the news

April 3, 2017. Crew members aboard the International Space Station will began conducting research to improve the way we grow crystals on Earth. The information gained from the experiments could speed up the process for drug development, benefiting humans around the world.

April 3, 2017. Researchers at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and Sandia National Laboratories working at the Joint BioEnergy Institute (JBEI) have resolved the protein structure of the enzyme LigM, which is utilized by the soil bacterium *Sphingomonas* to metabolize aryl compounds derived from lignin, the stiff, organic material that gives plants their structure.

April 5, 2017. Now Wei Liu and his colleagues at ASU's Biodesign Institute, along with a team led by Haitao Zhang and Vadim Cherezov of USC, have examined one promising drug target (AT2R, a critical cell receptor) in luminous detail, using an XFEL. AT2R belongs to a family of cell receptors known as GPCRs (for G-protein coupled receptor), the largest family of cell membrane receptors in the human genome.

April 10, 2017. Using several spectroscopic techniques, scientists at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) found that the element berkelium breaks form with its heavy element peers by taking on an extra positive charge when bound to a synthetic organic molecule. The researchers were able to provide even more confirmation utilizing X-ray crystallography at Berkeley Lab's Advanced Light Source, a DOE Office of Science User Facility.

April 10, 2017. Scientists have analyzed a mechanism that protects biomolecules such as DNA against damage by light. They observed how the energy of incoming photons can be absorbed by the molecule without destroying important bonds. The experiments took place at the Linac Coherent Light Source (LCLS) free-electron laser in California as well as the BESSY II synchrotron source at the HZB in Berlin.

April 12, 2017. A Lawrence Berkeley National Laboratory (Berkeley Lab) researcher, Banumathi Sankaran, worked as part of a multi-institutional team to map a key viral protein called NS5. Necessary to virus reproduction, NS5 contains two enzyme activities: one reduces the body's ability to mount an immune response against infection and the other helps start the genetic replication process. The work was led by Indiana University???s Cheng Kao and Pingwei Li at Texas A&M University (TAMU).

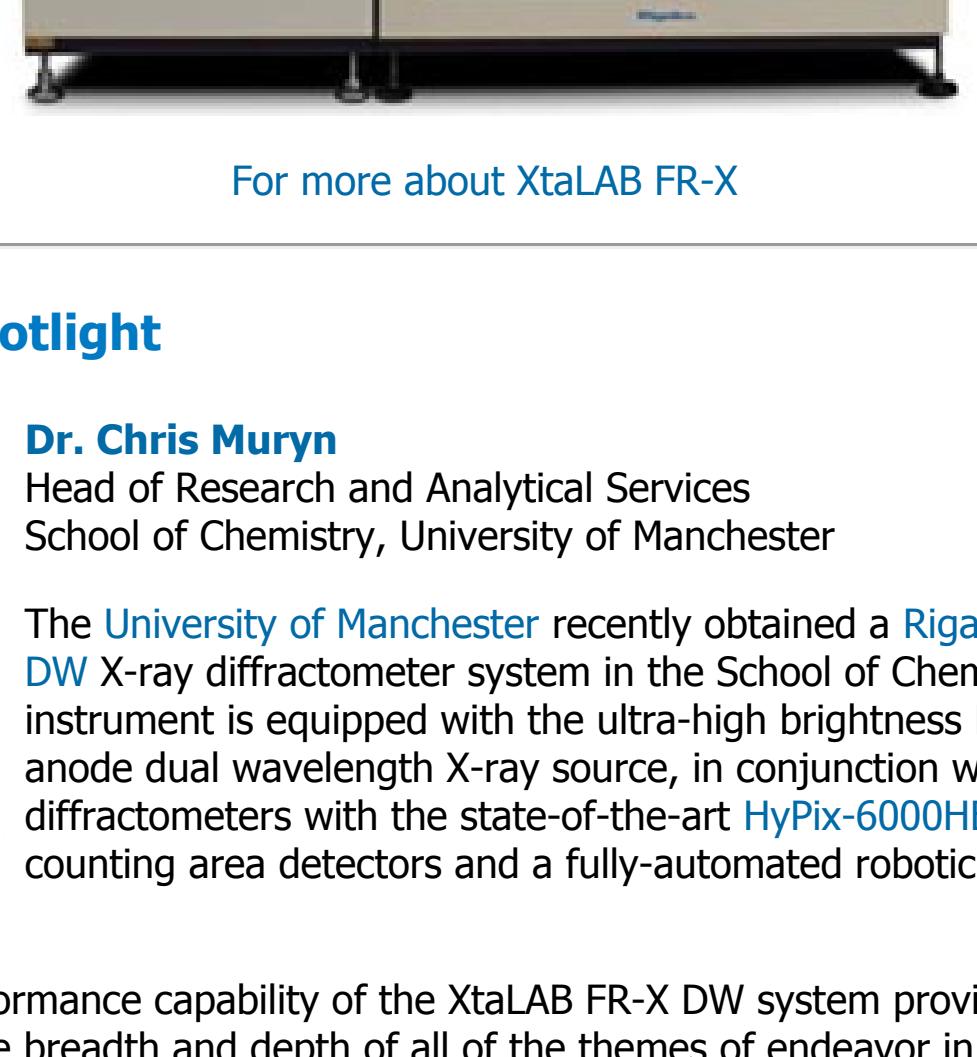
April 16, 2017. Researchers have come up with a new way to extract water from thin air. The new approach makes use of a substance called an MOF, a metal-organic framework. As the name suggests, these are materials made of metals mixed with organic compounds. Powders made from MOFs are very porous, so researchers have proposed using them to store hydrogen or methane fuels, or to capture carbon dioxide.

April 18, 2017. US scientists have discovered a chemical called Piperlongumine (PL) in a pepper plant, called long pepper, that has anti-cancer properties and whose medicinal properties date back thousands of years. Using X-ray crystallography, the researchers were able to create molecular structures that showed how the chemical is transformed after being ingested.

April 21, 2017. A team of researchers affiliated with Temple University and Argonne National Laboratory has developed a way to observe material restructuring at the atomic scale in real time. The method involved combining a small-angling X-ray scattering technique with molecular modeling software to track in precise detail the oxidation process of iron oxide nanoparticles.

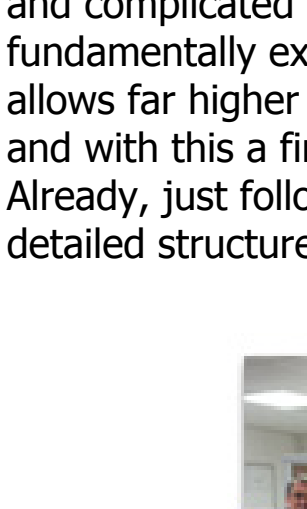
Product spotlight: XtaLAB FR-X

The XtaLAB FR-X system includes a VariMax optic coupled with the FR-X rotating anode generator. The FR-X is the most intense home lab X-ray source in the world and enables data collection on the widest range of protein crystal samples. It delivers 2.5 times higher flux compared to the MicroMax-007 HF rotating anode generator but shares the same microfocus 70 µm focal spot size. When coupled with Rigaku's VariMax optics, the FR-X delivers the highest brilliance for any commercially available rotating anode. As a result, it is possible to collect diffraction data for samples where no diffraction can be seen using a conventional rotating anode or sealed tube source.



For more about XtaLAB FR-X

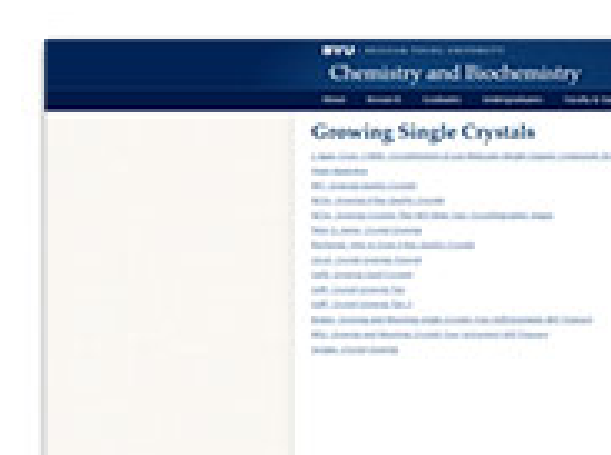
Lab in the spotlight

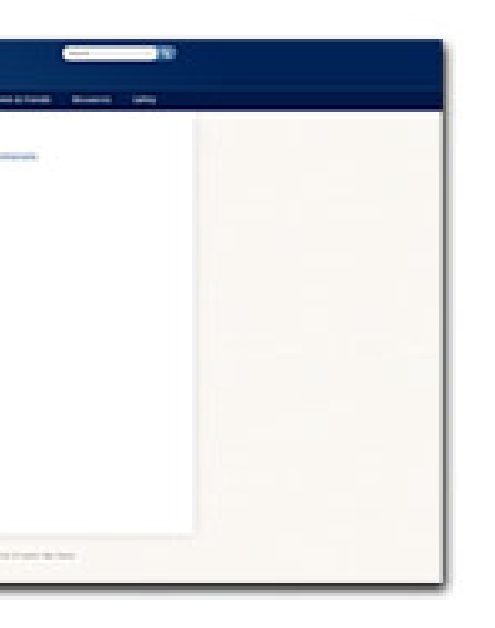


Dr. Chris Muryn
Head of Research and Analytical Services
School of Chemistry, University of Manchester

The University of Manchester recently obtained a Rigaku XtaLAB FR-X DW X-ray diffractometer system in the School of Chemistry. The instrument is equipped with the ultra-high brightness FR-X rotating anode dual wavelength X-ray source, in conjunction with dual diffractometers with the state-of-the-art HyPix-6000HE hybrid photon counting area detectors and a fully-automated robotic crystal handling system.

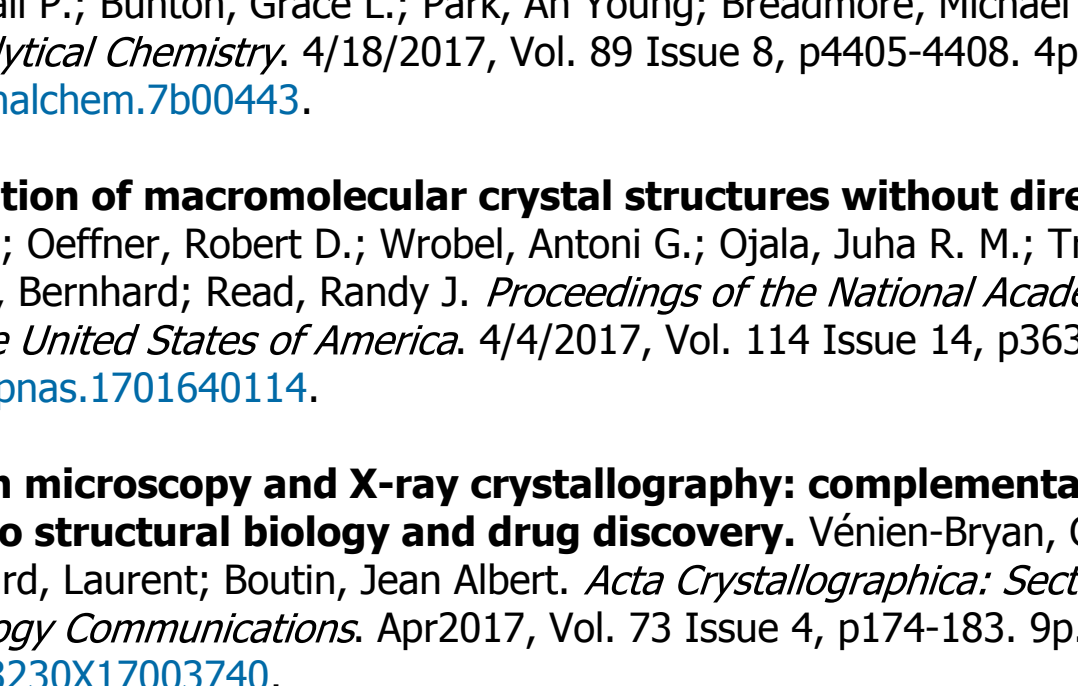
The ultimate performance capability of the XtaLAB FR-X DW system provides first class support across the breadth and depth of all of the themes of endeavor in the University of Manchester: world-leading research, for instance, in the areas of catenanes, rotaxanes, molecular knots and molecular motors, molecular magnetism, metal-organic framework materials and radiochemistry, etc. Throughout these research areas, – many with large and complicated molecular assemblies, the available crystals are very small and therefore fundamentally extremely weakly diffracting. The performance of the XtaLAB FR-X DW allows far higher resolution definitive structure-elucidation in these complicated materials and with this a finer understanding of important structure / function relationships. Already, just following installation and commissioning, the new equipment is allowing the detailed structure elucidation of as many as 20 new material structures, per day.





Useful link: Crystal growing

A very nice collection of links to small molecule crystal growing information from the Brigham Young University Chemistry Department website, compiled by the XRD Facility Manager, Dr. Stacey J. Smith.



Selected recent crystallographic papers

3D Printed Micrometer-Scale Polymer Mounts for Single Crystal Analysis. Macdonald, Niall P.; Bunton, Grace L.; Park, Ah Young; Breadmore, Michael C.; Kilah, Nathan L. *Analytical Chemistry*. 4/18/2017, Vol. 89 Issue 8, p4405-4408. 4p. DOI: 10.1021/acs.analchem.7b00443.

***Ab initio* solution of macromolecular crystal structures without direct methods.** Mccoy, Airlie J.; Oeffner, Robert D.; Wrobel, Antoni G.; Ojala, Juha R. M.; Tryggvason, Karl; Lohkamp, Bernhard; Read, Randy J. *Proceedings of the National Academy of Sciences of the United States of America*. 4/4/2017, Vol. 114 Issue 14, p3637-3641. 5p. DOI: 10.1073/pnas.1701640114.

Cryo-electron microscopy and X-ray crystallography: complementary approaches to structural biology and drug discovery. Vénien-Bryan, Catherine; Li, Zhuolun; Vuillard, Laurent; Boutin, Jean Albert. *Acta Crystallographica: Section F, Structural Biology Communications*. Apr2017, Vol. 73 Issue 4, p174-183. 9p. DOI: 10.1107/S2053230X17003740.

NIST Standard Reference Material 3600: Absolute Intensity Calibration Standard for Small-Angle X-ray Scattering. Allen, Andrew J.; Zhang, Fan; Kline, R. Joseph; Guthrie, William F.; Ilavsky, Jan. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p462-474. 12p. DOI: 10.1107/S1600576717001972.

Accurate Bond Lengths to Hydrogen Atoms from Single-Crystal X-ray Diffraction by Including Estimated Hydrogen ADPs and Comparison to Neutron and QM/MM Benchmarks. Dittrich, Birger; Lübben, Jens; Mebs, Stefan; Wagner, Armin; Luger, Peter; Flaig, Ralf. *Chemistry - A European Journal*. 4/3/2017, Vol. 23 Issue 19, p4605-4614. 10p. DOI: 10.1002/chem.201604705.

Jumping Crystals of Pyrene Tweezers: Crystal-to-Crystal Transition Involving π/ π-to-CH/ π Assembly Mode Switching. Shibuya, Yoshiki; Itoh, Yoshimitsu; Aida, Takuzo. *Chemistry - An Asian Journal*. 4/4/2017, Vol. 12 Issue 7, p811-815. 5p. DOI: 10.1002/asia.201700083.

The effect of X-ray irradiation on formation and decay of the incommensurate phase in $TlInS_2$ crystals. Nikolaienko, A. V.; Zloi, O. S.; Isaiev, M. V.; Gololobov, Yu. P.; Borovoy, N. A. *Physica Status Solidi (B)*. Apr2017, Vol. 254 Issue 4, pn/a-n/a. 5p. DOI: 10.1002/pssb.201600340.

Dynamic breathing effect in metal-organic frameworks: Reversible 2D-3D-2D-3D single-crystal to single-crystal transformation. Mendes, Ricardo F.; Almeida Paz, Filipe A. *Inorganica Chimica Acta*. Apr2017, Vol. 460, p99-107. 9p. DOI: 10.1016/j.ica.2016.09.037.

Crystal structures and enhanced luminescence of Zn(II) and Cd(II) complexes containing conjugated organic ligands. Sun, L.; Zhang, W.; Ma, J.; Gao, Y.; Xu, N.; Pan, C.; Lu, T.; Hu, X.; Jin, F. *Russian Journal of Coordination Chemistry*. Apr2017, Vol. 43 Issue 4, p252-259. 8p. DOI: 10.1134/S1070328417040078.

Supramolecular architectures and crystal structures of gold(III) compounds with semicarbazones. Gatto, Claudia C.; Lima, Iariane J.; Chagas, Marcio A. S. *Supramolecular Chemistry*. Apr2017, Vol. 29 Issue 4, p296-307. 12p. DOI: 10.1080/10610278.2016.1227440.

Structure–Property Relations and Polymorphism in Compressed Methylamines. Podsiadlo, Marcin; Olejniczak, Anna; Katrusiak, Andrzej. *Crystal Growth & Design*. 4/5/2017, Vol. 17 Issue 4, p2218-2222. 5p. DOI: 10.1021/acs.cgd.7b00203.

A Stable, Soluble, and Crystalline Supramolecular System with a Triplet Ground State. Futagoishi, Tsukasa; Aharen, Tomoko; Kato, Tatsuhisa; Kato, Azusa; Ihara, Toshiyuki; Tada, Tomofumi; Murata, Michihisa; Wakamiya, Atsushi; Kageyama, Hiroshi; Kanemitsu, Yoshihiko; Murata, Yasujiro. *Angewandte Chemie*. 4/3/2017, Vol. 129 Issue 15, p4325-4329. 5p. DOI: 10.1002/ange.201701212.

Two unusual isoflavonoids from *Campylotropis hirtella* – A new biosynthesis route of flavonoids. Ma, Jiahui; Zhang, Jinghua; Shen, Zhengwu. *Tetrahedron Letters: International Organ for the Rapid Publication of Preliminary Communications in Organic Chemistry*. Apr2017, Vol. 58 Issue 15, p1462-1466. 5p. DOI: 10.1016/j.tetlet.2017.02.080.

Data mining of iron(II) and iron(III) bond-valence parameters, and their relevance for macromolecular crystallography. Zheng, Heping; Langner, Karol M.; Hou, Jing; Minor, Wladek; Kowiel, Marcin; Shields, Gregory P.; Allen, Frank H.; Murshudov, Garib. *Acta Crystallographica Section D: Structural Biology*. Apr2017, Vol. 73 Issue 4, p316-325. 9p. DOI: 10.1107/S2059798317000584.

The metalation of hen egg white lysozyme impacts protein stability as shown by ion mobility mass spectrometry, differential scanning calorimetry, and X-ray crystallography. Sullivan, Matthew P.; Groessl, Michael; Meier, Samuel M.; Kingston, Richard L.; Goldstone, David C.; Hartinger, Christian G. *Chemical Communications*. 4/18/2017, Vol. 53 Issue 30, p4246-4249. 4p. DOI: 10.1039/c6cc10150j.

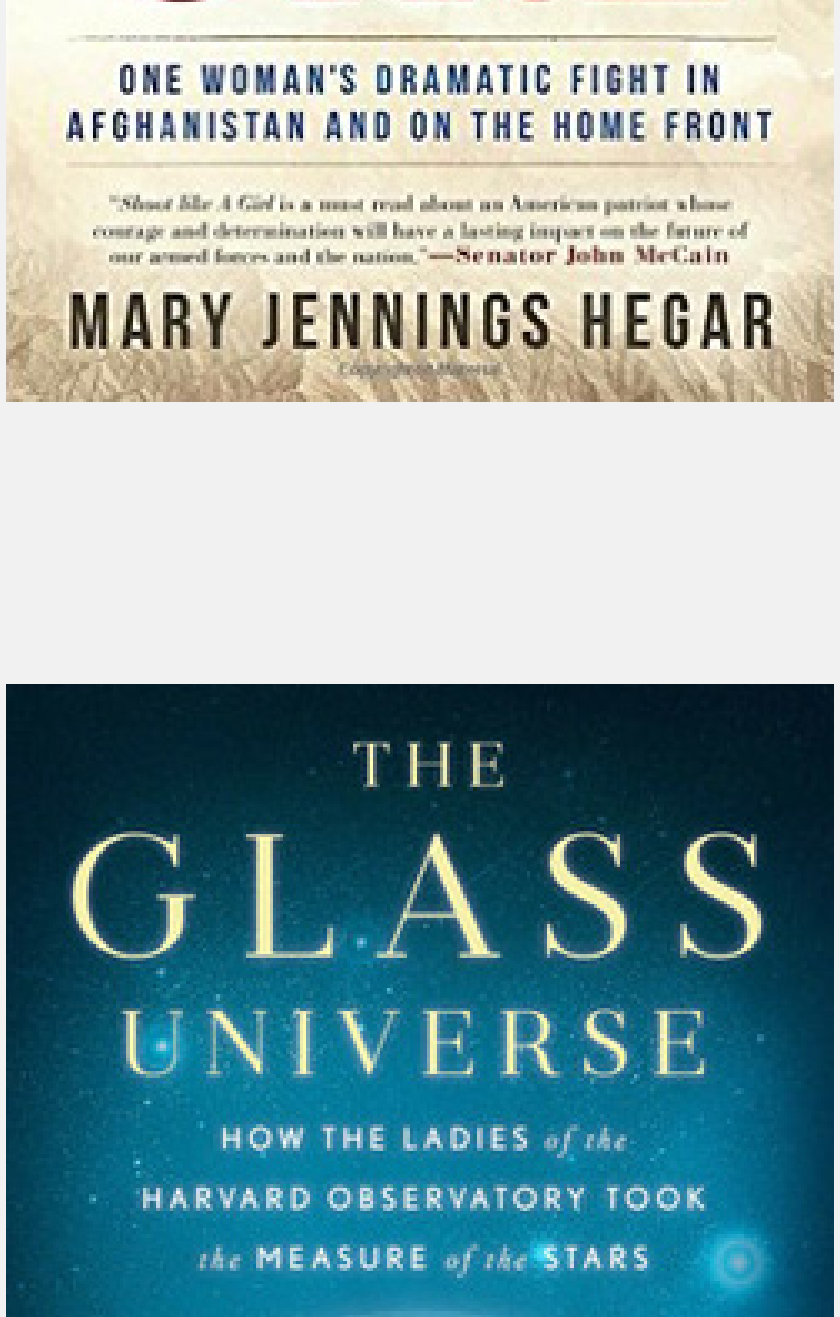
Elucidating the structure of an infectious protein. Zweckstetter, Markus; Requena, Jesús R.; Wille, Holger. *PLoS Pathogens*. 4/13/2017, Vol. 13 Issue 4, p1-6. 6p. DOI: 10.1371/journal.ppat.1006229.

Modeling disordered protein interactions from biophysical principles. Peterson, Lenna X.; Roy, Amitava; Christoffer, Charles; Terashi, Genki; Kihara, Daisuke. *PLoS Computational Biology*. 4/10/2017, Vol. 13 Issue 4, p1-28. 28p. DOI: 10.1371/journal.pcbi.1005485.

Quantitative evaluation of statistical errors in small-angle X-ray scattering measurements. Sedlak, Steffen M.; Bruetzel, Linda K.; Lipfert, Jan. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p621-630. 9p. DOI: 10.1107/S1600576717003077.

Insights on the structural dynamics of *Leishmania braziliensis* Hsp90 molecular chaperone by small angle X-ray scattering. Seraphim, Thiago V.; Silva, Kelly P.; Dores-Silva, Paulo R.; Barbosa, Leandro R.S.; Borges, J??lio C. *International Journal of Biological Macromolecules*. Apr2017, Vol. 97, p503-512. 10p. DOI: 10.1016/j.ijbiomac.2017.01.058.

Book review



***Shoot Like a Girl: One Woman's Dramatic Fight in Afghanistan and on the Home Front* by Mary Jennings Hegar, ISBN 978-1-101-98843-5**

Mary Jennings Hegar's memoir about her time in the U.S. Air Force and California National Guard is a must-read. In it, she shares her experience as a woman in the United States Armed Forces.

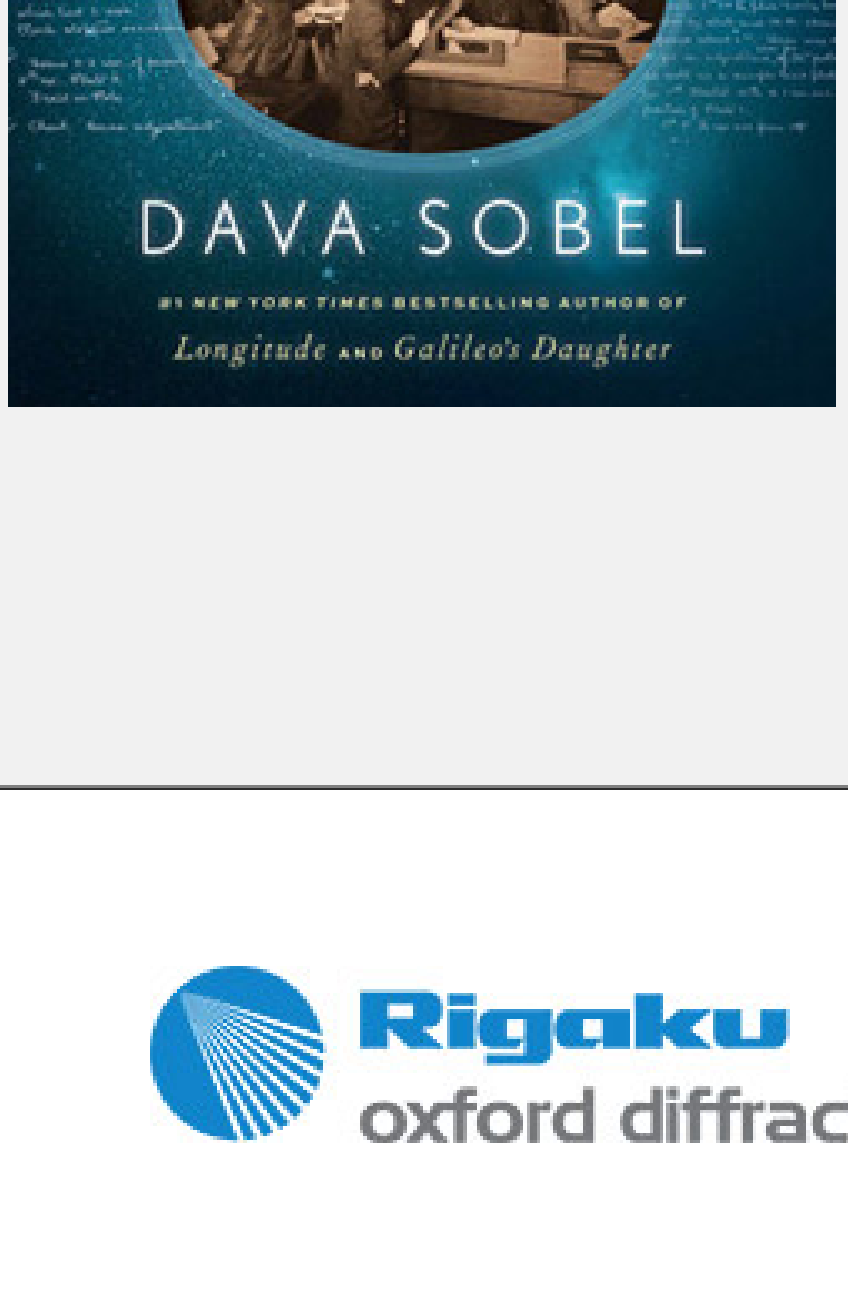
Her story isn't about what she was able to achieve in spite of being a woman, but rather what she was able to achieve despite being subjected to the abuse and prejudice aimed toward women like herself in the military.

She eloquently mixes the good with the bad with the ugly, giving enough personal detail to make her narrative compelling, but not so much that it belies the point at hand. She covers her abuses, at the hands of both a military doctor and her first husband. But she also covers her triumphs—moments shaped by trust and comradery, including the circumstances by which she earned a Purple Heart.

It is partly thanks to Mary Jennings Hegar that women are now allowed to fight in active combat. After her retirement from the military, Hegar joined the ACLU lawsuit to further gender equality in the military, which resulted in the removal of the sexist and outdated policy.

Part of what makes the book feel so authentic is the occasional blackout text, where the Department of Defense deemed certain details not fit for public consumption.

Shoot Like a Girl was a quick, cleverly written and honest read. I enjoyed it immensely, and I would recommend it to anyone with an interest in dogs, guns, the military, or strong female role models.



***The Glass Universe: How the Ladies of the Harvard Observatory Took the Measure of the Stars* by Dava Sobel, ISBN 978-0-670-01695-2**

When we think of the scientists and astronomers who studied the far reaches of our universe, men like Galileo Galilei and Stephen Hawking often come to mind. But Dava Sobel's latest work tells the untold story of the women who worked at the Harvard Observatory during the late 19th and early 20th centuries, mapping the stars and paving the way for future generations of astronomers and astrophysicists to study the mysteries of our universe.

Sobel begins her narrative with Anna Palmer Draper, the recently widowed Manhattan socialite and benefactor of the National Academy of Sciences who came to Harvard following the death of her husband to pursue her true love of the stars. She worked with Dr. Edward Pickering of the Harvard College Observatory.

Anna Draper established the Henry Draper Memorial, a means by which she could funnel her considerable funds into the observatory's coffers, fueling Pickering's research. Draper's deceased husband had desired to photograph the spectra of the stars, and it became her pet project to see his unfulfilled dream achieved. She donated numerous pieces of equipment to the observatory that would be used by generations of female researchers to come.

One of these researchers started out as Dr. Pickering's maid. Williamina Paton Stevens Fleming went from dusting bookshelves to establishing a system for classifying stars by their spectra. She worked as a female computer for the Harvard Observatory (in the 1800s, men preferred to have a woman do the math—not much had changed 70 years later, when women were doing most of the calculations for the Apollo missions at NASA). Fleming was also a curator of astronomical photographs at Harvard—a highly coveted position.

But Draper and Fleming are only two of the incredible women who contributed to the Harvard Observatory's successful ventures into studying the stars, and it would do these women, and Ms Sobel, a disservice if I were to further discuss them here. If you want more (and you should), read *The Glass Universe*.

Review by Jeanette S. Ferrara, MA

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