Crystallography Times

Crystallography Newsletter
Volume 9, No. 12, December 2017

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In this issue:

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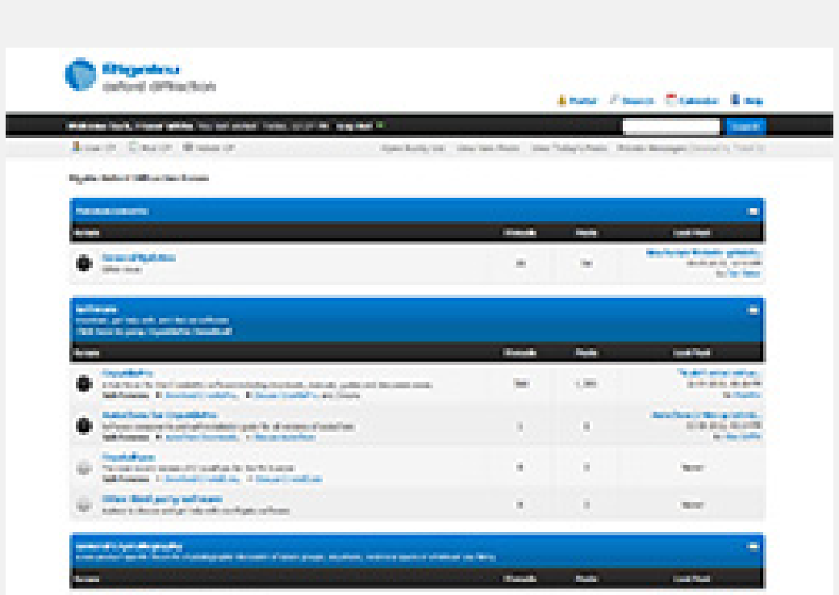
Rigaku Oxford Diffraction LinkedIn group shares information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories. You can also catch up on the latest newsletter or Rigaku Journal issue. We also hope that you will share information about your own research and laboratory groups.

Rigaku 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 CrysAlis^{Pro} software for single crystal data processing.

We look forward to seeing you on there soon.

Rigaku Reagents:
The Berkeley Screen

Rigaku Reagents is excited to announce the launch of our new screen, The Berkeley Screen!

Do you have that "go to" screen that you use to set up all of your trials? Are you having a difficult time getting crystals? Well, try the new Berkeley Screen! It has proven to provide crystals. The Berkeley Screen was developed by researchers at the Berkeley Center for Structural Biology at the Advanced Light Source of Lawrence Berkeley National Laboratory 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. Try our new 96 formulations and see for yourself!

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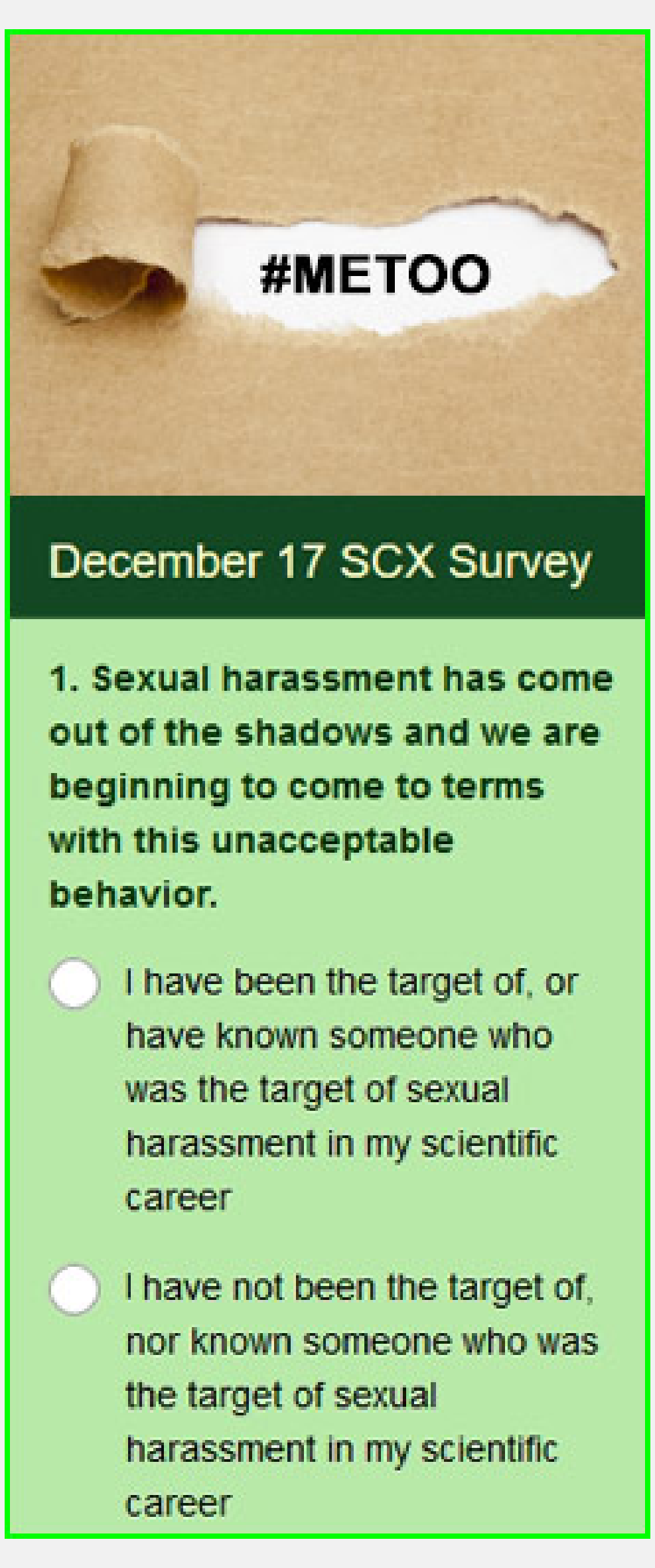
Survey of the month



December 17 SCX Survey

1. Sexual harassment has come out of the shadows and we are beginning to come to terms with this unacceptable behavior.

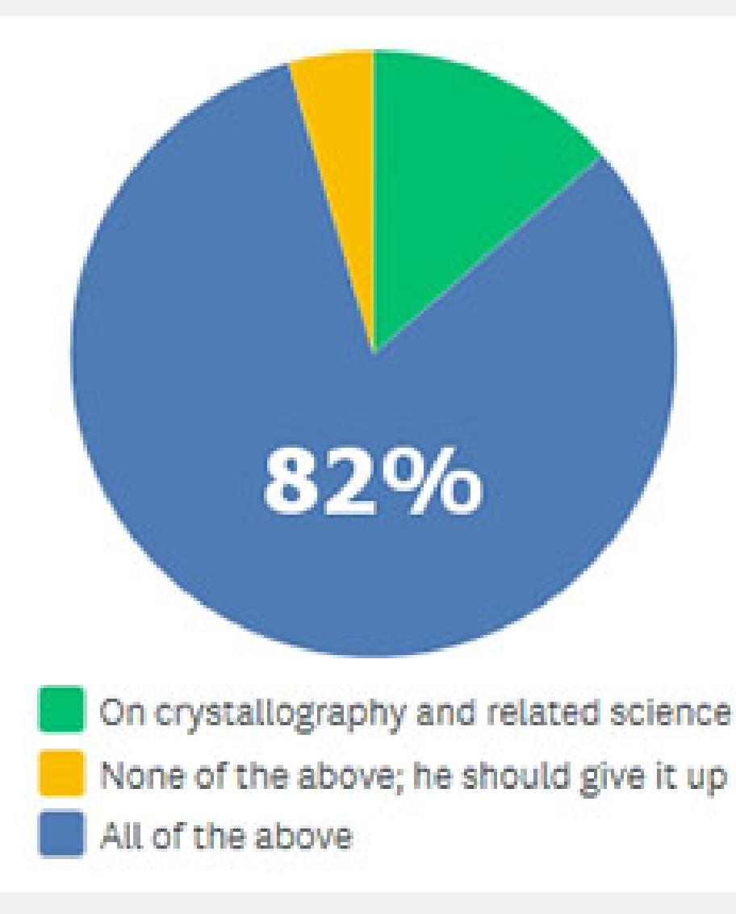
○ I have been the target of, or have known someone who was the target of sexual harassment in my scientific career

○ I have not been the target of, nor known someone who was the target of sexual harassment in my scientific career

Take the Survey

Last month's survey

The book editor should review books:



Videos of the month

Below is a link to this year's entries for the "Dance Your Ph.D." Contest. You'll find some of these funny and some rather thought provoking. Enjoy.

Watch the Video

And along the lines of making you laugh, then making you think here is a link to the 27th First Annual Ig Nobel Awards held this past September. This year???s keyword is Uncertainty and, as always, Miss Sweetie Pooh steals the show.

Watch the Video

Upcoming events

NESBA: The Resolution Revolution in cryoEM: Potential for Drug Discovery
Mar 16, 2018 in Waltham, MA, USA

International Small Angle Scattering Conference
Oct 7 – 12, 2018 in Traverse City, MI, USA

See full list >

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Crystallography in the news

December 4, 2017. Using X-ray diffraction, researchers in Russia, Germany and France are the first to have succeeded in determining the detailed structure of a light-sensitive membrane protein called channelrhodopsin 2, which is employed in optogenetics to control nerve cells with light.

December 8, 2017. Scientists at DESY have developed a new method that enables automated and fast screening of promising drug candidates. This novel technique, called mix-and-diffuse serial synchrotron crystallography, can image the interaction of potential drug targets with drug candidates or other molecules. In mix-and-diffuse serial synchrotron crystallography, protein crystals are mixed with a solution of a drug candidate and X-rayed on a tape running through the X-ray beam.

December 11, 2017. Scientists at the University of Copenhagen, led by the Spanish Professor Guillermo Montoya, are investigating the molecular features of different molecular scissors of the CRISPR-Cas system to shed light on the so-called "Swiss-army knives" of genome editing. Using X-ray crystallography, Montoya and colleagues have unveiled the high-resolution structure of Cpf1 and Cas9 to better understand their working mechanism, including the target DNA recognition and cleavage.

December 13, 2017. A new research initiative by the University of Maryland's Institute for Bioscience and Biotechnology Research (IBBR) and the University of Pittsburgh could finally uncover how T-cells—the "killer cells" that defend the body from microbes—are alerted to hazardous invaders in the body. Funded by a $3.7 million grant from the National Institutes of Health (NIH), the research will be the first to combine X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy for a unique view of the cell's alert system, which could lead to innovative therapeutics to fight viruses and tumors.

December 15, 2017. X-ray analytical instrumentation provider Rigaku Corporation has opened a new office in the Frankfurt Rhine-Main region. The new facility is home to a large and well-equipped application development and demonstration facility, complete with extensive sample preparation and wet chemistry labs.

December 15, 2017. Industry and agriculture generate vast quantities of methane, a potent greenhouse gas. However, marine microbes also represent an important source although exactly how is entangled in the "ocean methane paradox." Now, US researchers have used X-ray crystallography to explain it. Scientists from Massachusetts Institute of Technology and the University of Illinois at Urbana-Champaign have determined the structure of an enzyme that generates a precursor to methane.

December 15, 2017. During a Wellcome Trust-funded sabbatical at the National Institute of Genetics in Japan, Dr. Michael Webb from the Astbury Centre and School of Chemistry at the University of Leeds showed that pentyl pantothenamide targets the PanDZ complex, preventing *E. coli* from making Vitamin B5 and so starving it of the means to grow and resist the broad spectrum toxicity caused by the whole pantothenamide class. The team, which also involved scientists from the University of Hamburg, then used X-ray crystallography to map the structure of the complex.

Product spotlight: HyPix-6000HE

Rigaku Oxford Diffraction now offers the HyPix-6000HE Hybrid Photon Counting (HPC) detector. Like all HPCs, the HyPix-6000HE offers direct X-ray photon counting, single pixel point spread function and extremely low noise. The 100 micron pixel size allows better resolution of 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.

The advantage of direct detection found in the Hypix-6000HE is that no phosphor is required and the size of the pixel determines the point spread function rather than the blooming that occurs on detectors with a phosphor. This means that reflections will be sharper and profile analysis will not require incorporating additional pixels to compensate for phosphor blooming leading to less experimental noise, such as air scatter, being incorporated into a reflection.

As opposed to monolithic detectors, such as CMOS-based CPADs, a hybrid detector separates the detection area from the read-out electronics. This means that the full area of a pixel is sensitive to incoming photons, with the charge being transmitted through an indium bump bond to a secondary readout pixel. In monolithic detectors, each pixel contains a detection area and an electronics area, with the electronics area being insensitive to incoming photons. Monolithic detectors used in crystallography often have a 30% dead area or detection-gap per pixel which occurs through the whole detector.

The HyPix-6000HE is the perfect detector for measuring diffraction from small and poorly diffracting samples due to the extremely low noise characteristics: you can count as long as you need to without the dark current or noise build up seen in other detectors. When your crystals diffract well, the high frame rate and Zero Dead Time mode mean that you can collect data extremely fast and accurately in a shutterless mode.

Features:

- Direct photon counting with no phosphor blooming
- Single pixel point spread function
- 100 µm x 100 µm pixel size
- Extremely low noise
- Frame rate up to 100 Hz
- Electronically gateable
- Radiation tolerant design

For more about the HyPix-6000HE >

Lab in the spotlight

We've spent a lot of time over the last few years highlighting laboratories around the world. Now we'd like to take the opportunity to tell you about the laboratories at Rigaku. We have three main application laboratories: Tokyo, Japan; Wrocław, Poland and The Woodlands, USA. The lab in Tokyo supports the XtaLAB Synergy and XtaLAB Synergy Custom products, the XtaLAB mini II and BioSAXS. The Wrocław lab supports the XtaLAB Synergy products with XtaLAB Synergy-S, XtaLAB Synergy-R and XtaLAB Synergy-DW, and supports the PX Scanner. Finally, The Woodlands lab parallels the Tokyo lab. Scientists come in from all over the world, and their samples are analyzed at one of the three sites by our team of top notch application scientists.

Above is the Haijima, Japan Application Lab. On the left are X-ray microscopy, thermal analysis and XRF instruments. Up front are a XtaLAB mini II and a MiniFlex, and on the right are the single crystal analysis bays. Along the middle, unseen, are powder and stress instruments.

Above is the newly renovated Wrocław, Poland Application Lab. From left to right we see an XtaLAB Synergy-S with Ag and Mo sources, and a Pilatus 300K CdTe detector, a Mo XtaLAB Synergy-R with an Atlas S2 detector and on the far right a Cu XtaLAB Synergy-R with a HyPix-6000HE.

Above is The Woodlands, USA Application Lab. On the far left is an XtaLAB Synergy Custom system configured with an ACTOR automatic sample changer. Just to the right of that is an unseen XtaLAB Synergy-S with Cu and Mo sources, and a HyPix-6000HE detector. In the center is an FR-X generator with a BioSAXS-2000 (behind the tube tower) and an AFC11/P200K in front. To the right of the FR-X bay is the imaging bay with a nano3DX and CT Lab. And, finally, to the far right is a MicroMax-007HF generator with an AFC11/P200K.

Useful links

Here are two links that I personally use all the time. The first is great for world travelers – this tool allows you trace the shortest routes from any point to any other point on the globe, or figure out far out of the way your favorite airline is taking you.

Great Circle Mapper >

The third brightest object in the night sky is the International Space Station and NASA will tell you where and when you can see it, if the weather cooperates. You can sign up to receive notifications at the link below for your location. We have Spot-the-Station parties on our cul-de-sac and the neighborhood kids love it.

Spot The Station >

Selected recent crystallographic papers

Synthesis and Electronic Structures of Heavy Lanthanide Metallocenium Cations. Conrad A. P. Goodwin, Daniel Reta, Fabrizio Ortu, Nicholas F. Chilton, and David P. Mills. *Journal of the American Chemical Society*. Article ASAP. Dec17. DOI: 10.1021/jacs.7b11535.

An acoustic on-chip goniometer for room temperature macromolecular crystallography. Burton, C. G.; Axford, D.; Edwards, A. M. J.; Gildea, R. J.; Morris, R. H.; Newton, M. I.; Orville, A. M.; Prince, M.; Topham, P. D.; Docker, P. T. *Lab on a Chip - Miniaturisation for Chemistry & Biology*. 12/21/2017, Vol. 17 Issue 24, p4225-4230. 6p. DOI: 10.1039/c7lc00812k.

Hierarchical clustering for multiple-crystal macromolecular crystallography experiments: the *ccCluster* program. Santoni, Gianluca; Zander, Ulrich; Mueller-Dieckmann, Christoph; Leonard, Gordon; Popov, Alexander. *Journal of Applied Crystallography*. Dec2017, Vol. 50 Issue 6, p1844-1851. 7p. DOI: 10.1107/S1600576717015229.

A peak-finding algorithm based on robust statistical analysis in serial crystallography. Hadian-Jazi, Marjan; Messerschmidt, Marc; Darmanin, Connie; Giewekemeyer, Klaus; Mancuso, Adrian P.; Abbey, Brian. *Journal of Applied Crystallography*. Dec2017, Vol. 50 Issue 6, p1705-1715. 10p. DOI: 10.1107/S1600576717014340.

The planispherical chamber: A parallax-free gaseous X-ray detector for imaging applications. Brunbauer, F.M.; Oliveri, E.; Resnati, F.; Ropelewski, L.; Sauli, F.; Thuiner, P.; van Stenis, M. *Nuclear Instruments & Methods in Physics Research Section A*. Dec2017, Vol. 875, p16-20. 5p. DOI: 10.1016/j.nima.2017.08.060.

Synthesis, structures and magnetic properties of two chiral mixed-valence iron(II,III) coordination networks. Xue, Yun-Shan; Tan, Xu; Zhou, Mengjie; Mei, Hua; Xu, Yan. D*alton Transactions: An International Journal of Inorganic Chemistry*. 12/21/2017, Vol. 46 Issue 47, p16623-16630. 8p. DOI: 10.1039/c7dt03411c.

Crystal structure of an anti-idiotype variable lymphocyte receptor. Collins, Bernard C.; Nakahara, Hiro; Acharya, Sharmistha; Cooper, Max D.; Herrin, Brantley R.; Wilson, Ian A. *Acta Crystallographica: Section F, Structural Biology Communications*. Dec2017, Vol. 73 Issue 12, p682-687. 5p. DOI: 10.1107/S2053230X1701620X.

Design, synthesis and crystallographic study of novel indole-based cyano derivatives as key building blocks for heteropolycyclic compounds of major complexity. García, Andrés C.; Abonía, Rodrigo; Jaramillo-Gómez, Luz M.; Cobo, Justo; Glidewell, Christopher. *Acta Crystallographica: Section C, Structural Chemistry*. Dec2017, Vol. 73 Issue 12, p1040-1049. 9p. DOI: 10.1107/S2053229617015789.

Structural, spectroscopic and thermal property studies of cobalt adipate tetrahydrate single crystals. Jumanath, E.C.; Pradyumnan, P.P. *Journal of Crystal Growth*. Dec2017, Vol. 479, p83-88. 6p. DOI: 10.1016/j.jcrysgro.2017.09.025.

Evidence for M1-Linked Polyubiquitin-Mediated Conformational Change in NEMO. Hauenstein, Arthur V.; Xu, Guozhou; Kabaleeswaran, Venkataraman; Wu, Hao. *Journal of Molecular Biology*. Dec2017, Vol. 429 Issue 24, p3793-3800. 8p. DOI: 10.1016/j.jmb.2017.10.026.

Protein extraction into the bicontinuous microemulsion phase of a Water/SDS/pentanol/dodecane winsor-III system: Effect on nanostructure and protein conformation. Hayes, Douglas G.; Ye, Ran; Dunlap, Rachel N.; Cuneo, Matthew J.; Pingali, Sai Venkatesh; O'neill, Hugh M.; Urban, Volker S. *Colloids & Surfaces B: Biointerfaces*. Dec2017, Vol. 160, p144-153. 10p. DOI: 10.1016/j.colsurfb.2017.09.005.

The Crystal Structure and Conformations of an Unbranched Mixed Tri-Ubiquitin Chain Containing K48 and K63 Linkages. Padala, Prasanth; Soudah, Nadine; Giladi, Moshe; Haitin, Yoni; Isupov, Michail N.; Wiener, Reuven. *Journal of Molecular Biology*. Dec2017, Vol. 429 Issue 24, p3801-3813. 13p. DOI: 10.1016/j.jmb.2017.10.027.

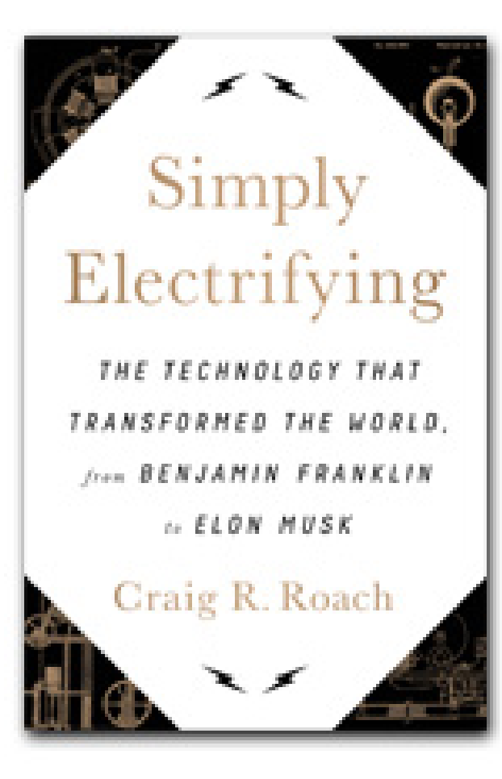
4-Methyl-1H-Indazole-5-Boronic acid: Crystal structure, vibrational spectra and DFT simulations. Dikmen, Gökhan. *Journal of Molecular Structure*. Dec2017, Vol. 1150, p299-306. 8p. DOI: 10.1016/j.molstruc.2017.08.097.

Polymorph-Dependent Green, Yellow, and Red Emissions of Organic Crystals for Laser Applications. Xu, Zhenzhen; Zhang, Zhiwei; Jin, Xue; Liao, Qing; Fu, Hongbing. *Chemistry - An Asian Journal*. 12/5/2017, Vol. 12 Issue 23, p2985-2990. 6p. DOI: 10.1002/asia.201701207.

Synthesis, crystal structure, physicochemical properties of hydrogen bonded supramolecular assembly of *N,N*-diethylanilinium-3, 5-dinitrosalicylate crystal. Rajkumar, M.; Chandramohan, A. *Journal of Molecular Structure*. Dec2017, Vol. 1149, p530-538. 9p. DOI: 10.1016/j.molstruc.2017.08.021.

Book review

Full disclosure: Dr. Roach is my brother-in-law and I was reluctant to print this review because I did not want give the impression of favoritism. However, this title appeared in JPMorgan's Next List for 2018 so I think it is reasonable to print Jeanette's review here.



***Simply Electrifying: The Technology that Transformed the World, from Benjamin Franklin to Elon Musk*, by Craig R. Roach*, BenBella Books, Inc., Dallas, 2017, 400 pages, ISBN: 978-1944648268**

A world without electricity would be a dark one indeed (both literally and figuratively). That's where Craig R. Roach starts *Simply Electrifying*: by asking the reader to imagine their world without the innumerable technologies that make our daily lives so much easier—technologies that predominantly run on electricity.

So who do we have to thank for this incredible energy that powers our lives? You've probably heard the story about how electricity was "discovered"—it involves founding father Benjamin Franklin, a kite, a key, and a lightning storm. Roach elaborates on the historical accuracy of this story and the impact of Franklin's experiment in his first chapter.

But what is electricity, really? When did it become something to be taken for granted? Where does it actually come from? How do we harness it? And who regulates how we use it?

These are all important questions Roach answers in his book—so even someone with little to no understanding of the "science" behind what electricity is (moving electrons), or the history of electricity (it's a rich one!), can read *Simply Electrifyin*g and walk away with a newfound knowledge of such a key aspect of their life.

Simply Electrifying is divided into five parts, or "ages" of electricity: The Age of Franklin, The Age of Edison, The Age of Big, The Age of Harm, and The Age of Uncompromising Belief.

Roach follows Franklin's discovery with James Watt's steam engine—an over two hundred year-old invention that cemented our modern dependence on coal-burning for electric power. Then, he takes a slight detour into the realm of the theoretical history of electricity: Faraday's Law of Induction and Maxwell's Equations.

After laying the groundwork, Roach details various inventors and their creations that employed the newfound electricity to power them, like Samuel Morse's telegraph and Thomas Edison???s light bulb. He touches on the Tesla-Edison AC/DC debate, and the mass deliverance of electricity to American homes.

Then Roach moves on to FDR's New Deal policies, which included bringing electricity to rural areas of the United States in an effort to combat unemployment. Hoover Dam and hydroelectricity, coal power, and Einstein's e = mc^2 all make appearances.

The dangers of electricity—namely the potential hazards of nuclear power and pollution from coal-powered plants—along with California's electricity crisis in the 1990s and the fall of Enron come next.

Finally, Roach ends with Obama's Clean Power Plan (how will it really impact the American public?), George Mitchell's shale gas revolution (fracking!) and the man many see as a real-life Tony Stark and the future of electricity: Elon Musk.

Simply Electrifying is not a light read—clocking in at 375 pages, not counting footnotes and indices—but it reads like one. Roach's prose hits the delicate balance between informative and compelling, covering all the bases in an objective and still interesting way.

Review by Jeanette S. Ferrara, MA

Rigaku Corporation
e-mail: info@rigaku.com
Tel: +[81] 3-3479-0618
FAX: +[81] 3-3479-6112

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

Rigaku China
e-mail: info@rigaku.com.cn
Tel: +[86] 010-88575768
FAX: +[86] 010-88575748

Rigaku Europe
e-mail: info@Rigaku.com
Tel: +[44] 1732 763 367
FAX: +[44] 1732 763 757