

Crystallography Newsletter

Volume 9, No. 10, October 2017

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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.

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: Spearlab foam dewars



Rigaku Reagents is now offering the popular Spearlab foam dewars. These polyethylene foam dewars are an effective way for handling liquid nitrogen and cryogenic materials. They are easy to handle, safe and durable!

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

Survey of the month



October 17 SCX Survey

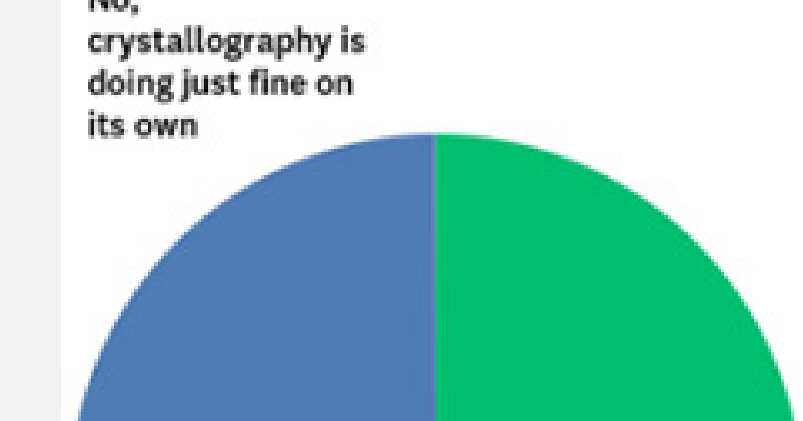
Do you find social media has enhanced your scientific career?

- Yes, it has made work life easier.
- No, it has made work life more difficult.
- What's social media?

[Take the Survey](#)

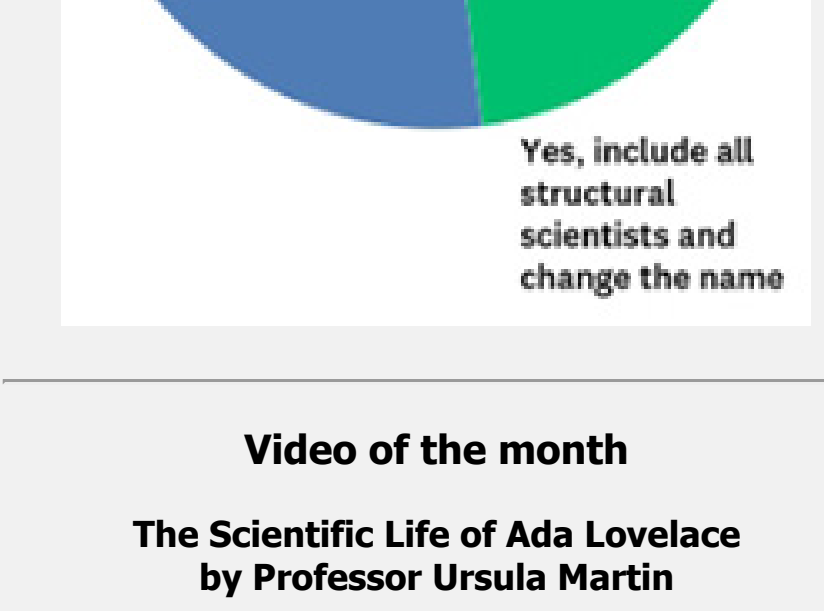
Last month's survey

Should the ACA consider changing its remit and its name to be inclusive of all structural science, including NMR, CryoEM etc?



Video of the month

The Scientific Life of Ada Lovelace by Professor Ursula Martin



October 10 is Ada Lovelace Day. Ada Lovelace (1815–1852) is recognized as the first software developer. There are many ways people have been celebrating this day over the years and here is one such lecture describing her life.

[Watch the Video](#)

Upcoming events

American Association of Pharmaceutical Scientists (AAPS) 2017
Nov 12 – 15, 2017 in San Diego, CA

25th Protein Structure Determination in Industry Meeting
Nov 12 – 14, 2017 in Cambridge, UK

CCDC CSD-Enterprise Workshop at Rigaku Oxford Diffraction
Nov 19, 2017 in The Woodlands, TX

CRYSTAL 31
Dec 3 – 7, 2017 in Bunker Bay, Western Australia

[See full list >](#)

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The CCDC CSD-Enterprise Workshop hosted by Rigaku Oxford Diffraction



The Cambridge Crystallographic Data Centre

The Cambridge Crystallographic Data Centre is sponsoring a workshop for anyone interested in learning more about the tools and features of the CCDC's CSD-Enterprise software. The workshop will be led by Dr. Amy Sarjeant and Dr. Shyam Vyas of the CCDC and will feature hands-on demonstrations of features from CSD-System and CSD-Materials.

Space is limited, so please register by October 30th >

Crystallography in the news

October 2, 2017. Aarhus University scientists have developed miniature antibodies (nanobodies) that provide a direct route for solving new X-ray crystal structures of protein complexes. They used a nanobody as the vehicle for introducing cryogenic atoms. This method to site-specifically label a nanobody with a heavy atom solves the phase problem.

October 3, 2017. Isabella L. Karle, Ph.D. died Oct. 3 at a hospice center in Arlington, Va. She was 95. A crystallographer, she received the National Medal of Science in 1995, bestowed by President Bill Clinton. After working on the Manhattan Project during World War II, Dr. Karle joined the NRL in 1946. Isabella Karle's other honors included the 1988 Gregori Aminoff Prize from the Royal Swedish Academy of Sciences, the 1993 Bower Award and Prize for Achievement in Science, and the Navy Distinguished Civilian Service Award. She was a member of the National Academy of Sciences.

October 4, 2017. The 2017 Nobel Prize in Chemistry has been awarded to Jacques Dubochet of the University of Lausanne, Joachim Frank of Columbia University, and Richard Henderson of the MRC Laboratory of Molecular Biology in Cambridge, England. They earned the prize for developing cryo-electron microscopy. The scientists will equally share the \$1.11 million award.

October 12, 2017. As part of an international research team, Jeff Donatelli, Peter Zwart and Kanupriya Pande of the Center for Advanced Mathematics for Energy Research Applications (CAMERA) at Lawrence Berkeley National Laboratory (Berkeley Lab) contributed key algorithms that helped achieve a goal first proposed more than 40 years ago – using angular correlations of X-ray snapshots from non-crystalline molecules to determine the 3D structure of important biological objects.

October 13, 2017. A team of Arizona State University scientists, led by Professor Alexandra Ros in the School of Molecular Sciences and the Biosign Center for Applied Structural Discovery, has been just the second user group to conduct experiments at the brand new European X-ray free electron laser facility (EuXFEL) in Hamburg, Germany. This \$1.5 billion facility is the third, and by far the most powerful, X-ray laser in the world. After ten years of construction, it opened for first experiments just a month ago.

October 16, 2017. The National Institutes of Health (NIH) has awarded \$6.5 million to Lawrence Berkeley National Laboratory (Berkeley Lab) to integrate existing synchrotron structural biology resources to better serve researchers. The grant will establish a center based at the Lab's Advanced Light Source (ALS) called ALS-ENABLE that will guide users through the most appropriate routes for answering their specific biological questions.

October 16, 2017. Scientists at the Department of Energy's Oak Ridge National Laboratory have performed neutron structural analysis of a vitamin B6-dependent protein, potentially opening avenues for new antibiotics and drugs to battle diseases such as drug-resistant tuberculosis, malaria and diabetes.

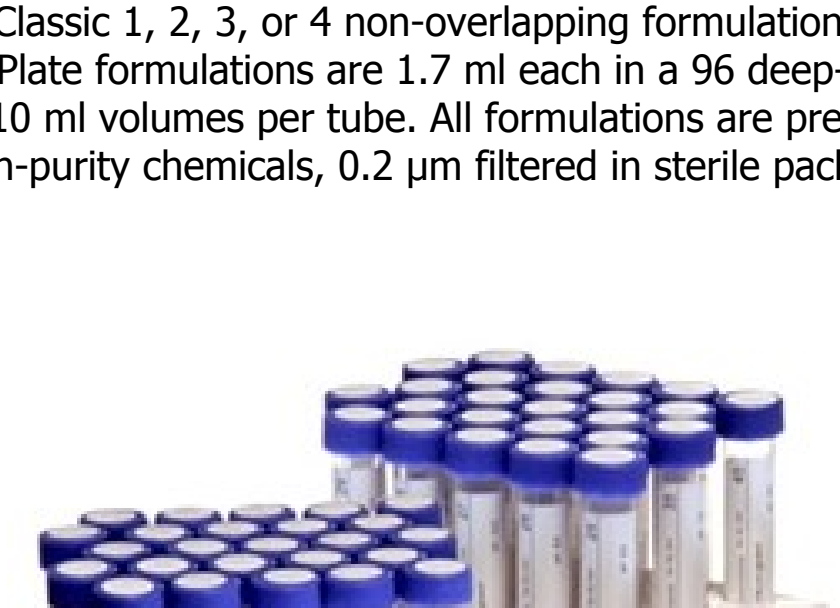
October 19, 2017. Robert Henry "Pete" Bragg, Jr., professor emeritus in the Department of Materials Science and Engineering in the College of Engineering at UC Berkeley, passed away on Oct. 3 at the age of 98. Bragg joined the Berkeley faculty in June 1969. Bragg was a leading expert in X-ray crystallography, X-ray diffraction and materials characterization.

Product spotlight: Wizard Classic crystallization screen series

The Wizard[™] Classic line of random sparse matrix screens is designed to increase your probability of producing crystals during the coarse screening phase when crystallizing biological macromolecules (proteins, nucleic acids, peptides, and combinations thereof).

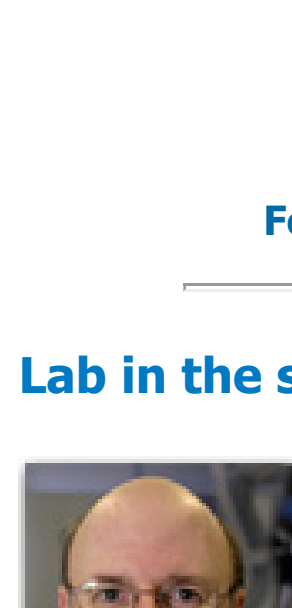
The Wizard Classic reagents are proven to be a highly effective starting point in the screening of biological macromolecules. The Wizard Classic formulations include a large range of crystallants, buffers, and salts covering a broad range of crystallization space at pH levels from pH 4.5 to pH 10.5.

Choose from Wizard Classic 1, 2, 3, or 4 non-overlapping formulations in matrix blocks or tubes. 96-Well Block Plate formulations are 1.7 ml each in a 96 deep-well matrix block plate. Tube sets are 10 ml volumes per tube. All formulations are prepared with ASTM type-1 water and high-purity chemicals, 0.2 µm filtered in sterile packaging.



[For more about Wizard Classic crystallization screens >](#)

Lab in the spotlight



The Linden Research Group
Prof. Dr. Anthony Linden
University of Zurich
Department of Chemistry

The Linden research group is interested in modelling the solid state structures of disordered molecular materials showing diffuse scattering, as well as in a broad range of questions in chemical crystallography.

The Determination of Disordered Crystal Structures from Diffuse Scattering
The aim of Professor Linden's work is to further develop the tools for analyzing such scattering and to investigate molecular materials with important properties. The research is intended to contribute readily accessible, methodological advances to a neglected and underdeveloped part of crystal structure analysis, which, unlike studies of ordered materials, is far from routine. The number of studies involving diffuse scattering from disordered molecular materials is very limited compared with that for ordered structures.

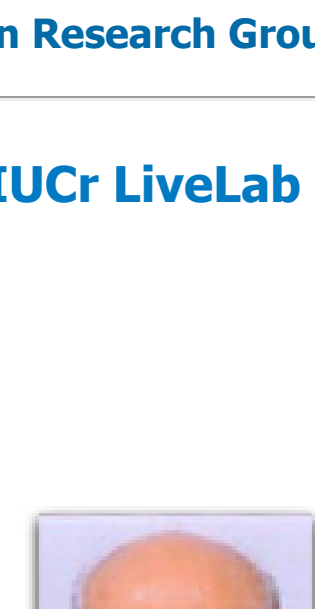
The modeling of the structures involves the use of computationally demanding genetic algorithms and Monte Carlo calculations. The measurement of diffuse diffraction data requires very bright light sources, such as those at the European Synchrotron Radiation Facility and the Institut Laue Langevin in Grenoble. Solutions to problems of disorder in materials are of interest internationally in the chemical industry, as in the cases of the recently postulated second polymorph of Aspirin and Pigment Red, both of which are economically significant materials. They are also of interest locally, as one focus of research at the University of Zurich is to develop molecular materials with interesting solid state stereochemistry that sometimes requires advanced diffuse scattering models to resolve.

Chemical Crystallography

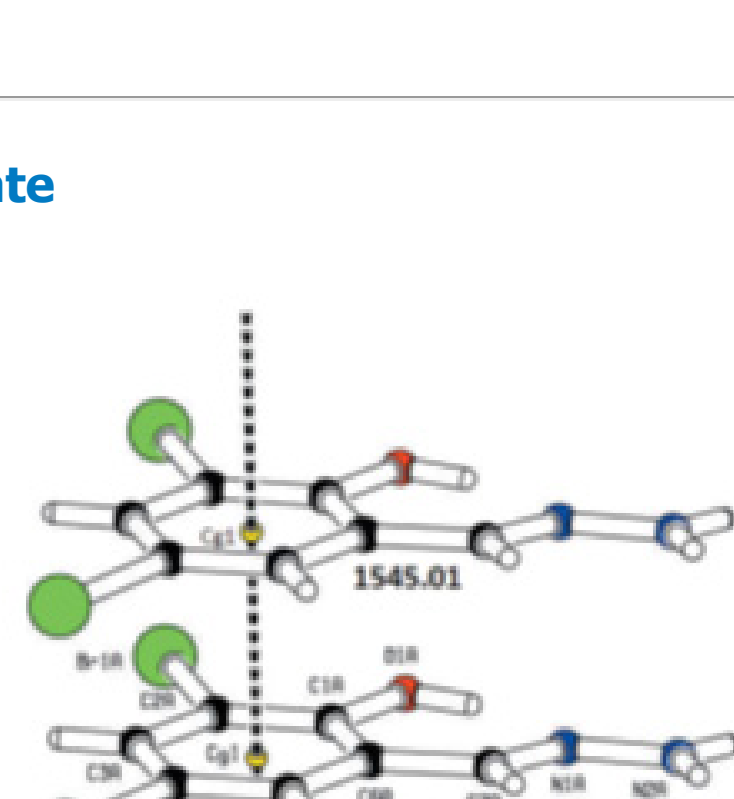
The Linden group has a general interest in molecular interactions and their relationship to structural properties. Single-crystal X-ray crystallography is used as the main investigative tool. Aspects of hydrogen bonding and how this drives the supramolecular and structural properties of materials is a key focus.

[The Linden Research Group >](#)

Rigaku IUCr LiveLab Update



Sushil K. Gupta



The first publication from the XtaLAB mini II installed at the Rigaku LiveLab at IUCr2017 in Hyderabad has been released:

(E)-2,4-Dibromo-6-(hydrazinylidenemethyl)phenol by Rayees A. Bhat, D. Kumar, Javed A. Ganaie, Ray J. Butcher and Sushil K. Gupta (2017) *IUCrData*, 2, x171386 <https://doi.org/10.1107/S2414314617013864>

The title compound, C₇H₆Br₂N₂O, was obtained from a condensation reaction of 3,5-dibromo-2-hydroxybenzaldehyde and hydrazine hydrate. The molecule is approximately planar, the largest deviation from the mean plane through all of the non-H atoms being 0.053(1) Å. The molecular conformation is stabilized by an intramolecular O—H...N hydrogen bond, generating an S(6) ring motif. In the crystal, intermolecular N—H...N and N—H...O hydrogen bonds link the molecules, forming chains parallel to the *b* axis. Molecules are further linked by ?????? stacking interactions, with centroid-centroid distances of 3.925(3)????3.926(3) Å, forming a three-dimensional network.

Useful link

[Final report of the IUCr Diffraction Data Deposition Working Group](#)
John R Hellinwell, Brian McMahon, Steve Androulakis, Marian Szebenyi, Loes Kroon-Batenburg, Tom Terwilliger, John Westbrook and Edgar Weckert

Selected recent crystallographic papers

High-Resolution Cryo-EM Maps and Models: A Crystallographer's Perspective. Wlodawer, Alexander; Li, Mi; Dauter, Zbigniew. *Structure*. Oct2017, Vol. 25 Issue 10, p1589-1597.e1. 1p. DOI: [10.1016/j.str.2017.07.012](https://doi.org/10.1016/j.str.2017.07.012).

Applications of dynamical theory of X-ray diffraction by perfect crystals to reciprocal space mapping. Punegov, Vasily I.; Pavlov, Konstantin M.; Karpov, Andrey V.; Faleev, Nikolai N. *Journal of Applied Crystallography*. Oct2017, Vol. 50 Issue 5, p1256-1266. 10p. DOI: [10.1107/S1600576717010123](https://doi.org/10.1107/S1600576717010123).

BioXTAS RAW: improvements to a free open-source program for small-angle X-ray scattering data reduction and analysis. Hopkins, Jesse Bennett; Gillilan, Richard E.; Skou, Soren. *Journal of Applied Crystallography*. Oct2017, Vol. 50 Issue 5, p1545-1553. 8p. DOI: [10.1107/S1600576717011438](https://doi.org/10.1107/S1600576717011438).

Cationic and Anionic Disorder in CZTSSe Kesterite Compounds: A Chemical Crystallography Study. Bais, Pierre; Caldes, Maria Teresa; Paris, Michaël; Guillot-Deudon, Catherine; Fertey, Pierre; Doméngès, Bernadette; Lafond, Alain. *Inorganic Chemistry*. 10/2/2017, Vol. 56 Issue 19, p11779-11786. 8p. DOI: [10.1021/acs.inorgchem.7b01791](https://doi.org/10.1021/acs.inorgchem.7b01791).

A new model for the description of X-ray diffraction from mosaic crystals for ray-tracing calculations. Schlesiger, Christopher; Anklam, Lars; Malzer, Wolfgang; Gnewkow, Richard; Kannigler, Birgit. *Journal of Applied Crystallography*. Oct2017, Vol. 50 Issue 5, p1490-1497. 7p. DOI: [10.1107/S1600576717012626](https://doi.org/10.1107/S1600576717012626).

Crystallography of Complex Forms: The Case of Ocular Sclerites. Vielzeuf, Daniel; Floquet, Nicole; Perrin, Jonathan; Tambuté, Eric; Ricolleau, Angèle. *Crystal Growth & Design*. Oct2017, Vol. 17 Issue 10, p5080-5097. 18p. DOI: [10.1021/acs.cgd.7b00087](https://doi.org/10.1021/acs.cgd.7b00087).

Towards a compact and precise sample holder for macromolecular crystallography. Papp, Gergely; Rossi, Christopher; Janocha, Robert; Sorez, Clement; Lopez-Marrero, Marcos; Astruc, Anthony; McCarthy, Andrew; Belrhali, Hassan; Bowler, Matthew W.; Cipriani, Florent. *Acta Crystallographica Section D: Structural Biology*. Oct2017, Vol. 73 Issue 10, p829-840. 11p. DOI: [10.1107/S2059798317013742](https://doi.org/10.1107/S2059798317013742).

FlexED8: the first member of a fast and flexible sample-changer family for macromolecular crystallography. Papp, Gergely; Felissaz, Franck; Sorez, Clement; Lopez-Marrero, Marcos; Janocha, Robert; Manjasetty, Babu; Gobbo, Alexandre; Belrhali, Hassan; Bowler, Matthew W.; Cipriani, Florent. *Acta Crystallographica Section D: Structural Biology*. Oct2017, Vol. 73 Issue 10, p841-851. 10p. DOI: [10.1107/S2059798317013596](https://doi.org/10.1107/S2059798317013596).

A zigzag path through quantum crystallography. Massa, Lou. *Structural Chemistry*. Oct2017, Vol. 28 Issue 5, p1293-1296. 4p. DOI: [10.1007/s11224-017-0960-9](https://doi.org/10.1007/s11224-017-0960-9).

Averaging of elastic constants for polycrystals. Blaschke, Daniel N. *Journal of Applied Physics*. 10/14/2017, Vol. 122 Issue 14, p145110-1-145110-6. 6p. 7 Charts. DOI: [10.1063/1.4993443](https://doi.org/10.1063/1.4993443).

Hybrid approach to structure modeling of the histamine H3 receptor: Multi-level assessment as a tool for model verification. Jonczyk, Jakub; Malawska, Barbara; Bajda, Marek. *PLoS ONE*. 10/05/2017, Vol. 12 Issue 10, p1-29. 29p. DOI: [10.1371/journal.pone.0186108](https://doi.org/10.1371/journal.pone.0186108).

The discovery and investigation of a crystalline solid solution of an active pharmaceutical ingredient. Patel, Mitulkumar A.; AbouGhaly, Mohamed H.H.; Chadwick, Keith. *International Journal of Pharmaceutics*. Oct2017, Vol. 532 Issue 1, p166-176. 11p. DOI: [10.1016/j.ijpharm.2017.08.101](https://doi.org/10.1016/j.ijpharm.2017.08.101).

Structural insights into the usage of boroxylate ions as molecular pins. Swiatkowski, Marcin; Kruszynski, Rafal. *Polyhedron*. Oct2017, Vol. 135, p265-277. 13p. DOI: [10.1016/j.poly.2017.07.011](https://doi.org/10.1016/j.poly.2017.07.011).

Large-scale crystallization and neutron crystallographic analysis of HSP70 in complex with ADP. Yokoyama, Takeshi; Ostermann, Andreas; Schrader, Tobias E.; Mizuguchi, Mineyuki. *Acta Crystallographica Section B: Structural Biology Communications*. Oct2017, Vol. 73 Issue 10, p555-559. 4p. DOI: [10.1107/S20523230X1701264X](https://doi.org/10.1107/S20523230X1701264X).

De novo design of covalently constrained mesosize protein scaffolds with unique tertiary structures. Bobo Dang, Haifan Wu; Mulligan, Vikram Khipple; Mravic, Marco; Yibing Wu; Lemmin, Thomas; Ford, Alexander; Silva, Daniel-Adriano; Baker, David; DeGrado, William F. *Proceedings of the National Academy of Sciences of the United States of America*. 10/10/2017, Vol. 114 Issue 41, p10852-10857. 6p. DOI: [10.1073/pnas.1710695114](https://doi.org/10.1073/pnas.1710695114).

Discovery of BAZ2A bromodomain ligands. Spiliotopoulos, Dimitrios; Wamhoff, Eike-Christian; Lolli, Graziano; Rademacher, Christopher; Caffisi, Amedeo. *European Journal of Medicinal Chemistry*. Oct2017, Vol. 139, p564-572. 9p. DOI: [10.1016/j.ejmech.2017.08.028](https://doi.org/10.1016/j.ejmech.2017.08.028).

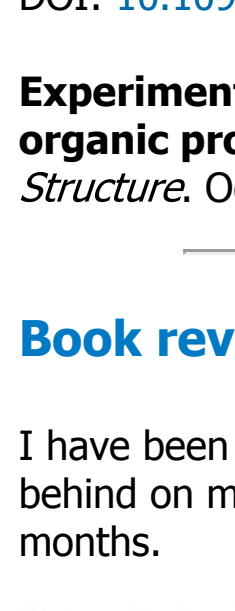
Structural basis of the PE???PPE protein interaction in Mycobacterium tuberculosis. Xin Chen; Hui-fu Cheng; Junwei Zhou; Chiu-yeung Chan; Kwok-fai Lau; Stephen Kwok-wing Tsui; Shannon Wing-ngor Au. *Journal of Biological Chemistry*. 10/13/2017, Vol. 292 Issue 41, p16880-16890. 11p. DOI: [10.1074/jbc.M117.802645](https://doi.org/10.1074/jbc.M117.802645).

Conserved threonine 1505 in the catalytic domain stabilizes mouse DNA methyltransferase 1. Kensaku Kanada; Kohei Takeshita; Isao Suetake; Shoji Tajima; Atsushi Nakagawa. *Journal of Biochemistry*. Oct2017, Vol. 162 Issue 4, p271-278. 8p. DOI: [10.1093/jb/mvx024](https://doi.org/10.1093/jb/mvx024).

Experimental and computational studies on creatininium 4-nitrobenzoate – An organic proton transfer complex. Thirumurugan, R.; Anitha, K. *Journal of Molecular Structure*. Oct2017, Vol. 1146, p273-284. 12p. DOI: [10.1016/j.molstruc.2017.05.143](https://doi.org/10.1016/j.molstruc.2017.05.143).

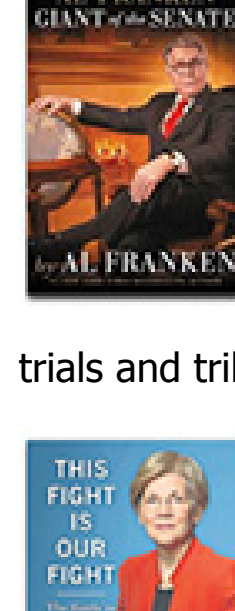
Book reviews

I have been focused on a number of recent titles that analyze current events so I am a bit behind on my reviews of science-oriented books. Here is what I???ve read the last few months.



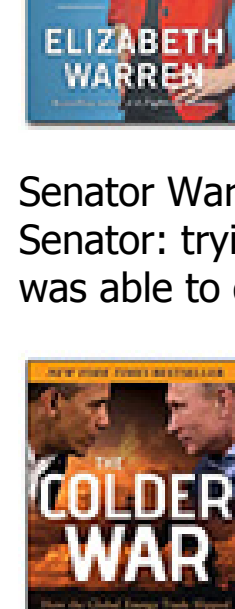
Al Franken, Giant of the Senate by Al Franken, Hachette Book Group, Inc. New York, 2017, 416 pp, ISBN-13: 978-1455540419.

Al Franken has not been funny since he became a politician—at least on purpose—until now. Here Senator Franken describes growing up in the Minneapolis suburb of St. Louis Park, becoming a comedian and making it on Saturday Night Live, becoming a United States Senator and finally a description of his time on the Hill. Interspersed in the narrative are the trials and tribulations we all face as Americans.



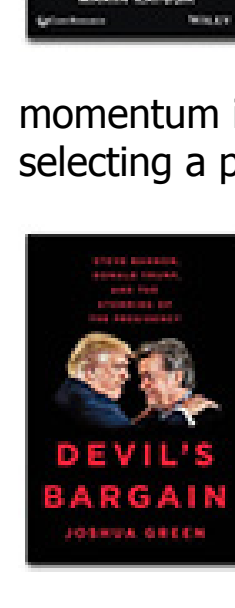
This Fight Is Our Fight: The Battle to Save America's Middle Class by Elizabeth Warren, Henry Holt and Co., New York, 2017, 352 pages, ISBN-13: 978-1250120618.

Senator Warren describes her life growing up in Oklahoma with her mother as breadwinner, getting into college, dropping out to have a family, then going back to school and ultimately becoming a lawyer. She had been teaching law for nearly 35 years when she was elected Senator in 2012. Senator Warren's book focuses on the issue she has tried to address as a United States Senator: trying to provide the lower classes with the tools to advance in society as she was able to do.



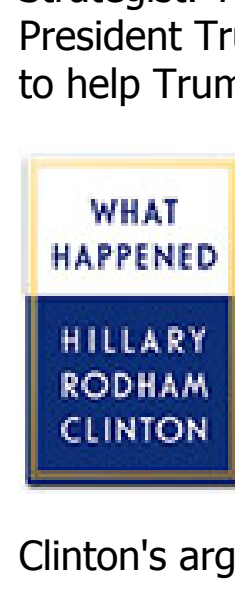
The Colder War: How the Global Energy Trade Slipped from America's Grasp by Marin Katusa, John Wiley & Sons, Hoboken, 2015, 272 pages, ISBN-13: 978-1118799949.

This book was recommended to me by a colleague. It describes in detail Putin's rise to power and the slow but gradual takeover of the world energy markets—oil, gas and uranium—by the Russian Federation. This book predates the 2016 election but one can see the need to maintain momentum in dominating world markets; e.g., thinking sanctions would be reduced by selecting a pro-Putin candidate and interfering in the 2016 election.



Devil's Bargain, Steve Bannon, Donald Trump and the Storming of the Presidency by Joshua Green, Penguin Press, New York, 2017, 288 pp, ISBN-13: 978-0735225022.

This is a short biography of Steve Bannon. It follows him from his early years in Catholic schools to his time in the US Navy and his work at Goldman-Sachs. Then it details his career in television and movie making, his tenure at Breitbart News and ending with his appointment as Chief Strategist. The author also provides a history of the relationship between Bannon and President Trump, and explains how Bannon was instrumental in restricting the campaign to help Trump with the 2016 election.



What Happened by Hillary Rodham Clinton, New York, 2017, 512 pp, ISBN-13: 978-1501175565.

You will either agree wholeheartedly with Secretary Clinton's analysis of why she lost the 2016 election or you will vehemently disagree. There is a lot of discussion about family and friends that could have been left out to focus more on the facts of the 2016 election. A volume two of this book will probably come out once the Muller investigation is complete and Clinton's arguments about Russian meddling in the election are verified.

Reviews by Joseph Ferrara
Deputy Director, X-ray Research Laboratory, Rigaku