# Crystallography Times

**Crystallography Newsletter**
Volume 11, No. 03, March 2019
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**In this issue:**


- Users' Meeting at the BCA
- Crystallography in the News
- Visit with Us
- Join ROD on LinkedIn
- Product Spotlight
- Wizard Cryo crystallization screen series
- Rigaku X-ray Forum
- Lab in the Spotlight
- Survey of the Month
- Last Month's Survey
- Useful Link
- Video of the Month
- Recent Crystallographic Papers
- Book Review


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**Visit with Us**

27th Annual Meeting of the German Crystallographic Society (DGK)
Leipzig, Germany, March 25 – 28, 2019

American Chemical Society National Meeting and Exposition (ACS Spring 2019)
Orlando, FL, March 31 – April 4, 2019

British Crystallographic Association Spring Meeting (BCA Spring Meeting 2019)
Nottingham, UK, April 15 – 18, 2019

Second Annual Industrial Biostructures America (IBA) Conference
La Jolla, California, May 19 – 21, 2019

102nd Canadian Chemistry Conference and Exhibition
Québec City, Canada, June 3 – 7, 2019

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**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.

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**Rigaku Reagents:**
**Wizard Cryo™ crystallization screen series**



## Users' Meeting at the BCA

At the BCA Spring meeting in Nottingham this year we will be hosting an afternoon users' meeting featuring talks on both single-crystal and powder X-ray diffraction topics. Please join us on Thursday 18th April in the afternoon to learn about the latest software and hardware developments. Chat about issues you face in pursuit of your research with our staff and user community over tea, coffee and biscuits.

Places are limited and we need to know numbers in advance so please sign up at the following link as early as possible.

**Register for European Users' Meeting**

Please plan to turn up 10 – 15 minutes before the start time, 2 pm, so that we can register you and start on time. Speakers will include Mathias Meyer and Fraser White from Rigaku and Keith Tame from SciMed.

We look forward to see you there.

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## Crystallography in the News

**March 1, 2019.** New research sheds light onto how different bacterial species can build complex nano-harpoons with different protein building blocks. Bacteria use these harpoons, called Type VI secretion systems, to inject toxins into nearby cells. Researchers from the University of Sheffield found that while the proteins varied, there were structurally similar portions that interacted with the machinery.

**March 4, 2019.** National Institute of Environmental Health Sciences (NIEHS) researchers have discovered a possible explanation for why flavonoids, the healthy chemicals in many fruits and vegetables, may be so good for you. The scientists reported that quercetin, a flavonoid found in capers, dill, chili peppers, fennel, onions, and cranberries, specifically blocked the activity of a protein called IP6K that promotes the migration of cancer cells to different regions of the body.

**March 7, 2019.** Crystal-clear view of a key neuronal receptor opens door for new, targeted drugs. In a new study published in *Cell*, Bar-Ilan University researchers and collaborators report on their discovery of the intricate molecular mechanism that allows the guidance receptor Robo to react to signals in its environment, while avoiding premature activity that can lead to harmful outcomes.

**March 8, 2019.** GS-6207, a first-in-class HIV capsid (CA) inhibitor, has picomolar potency and a distinct pharmacokinetic and resistance profile that establishes it as a suitable candidate for a low-dose, long-acting subcutaneous administration to treat HIV infection. The study team used surface plasmon resonance and X-ray crystallography to evaluate how GS-6207 binds to HIV-1 CA hexamers.

**March 12, 2019.** Harvard structural biologist Stephen C. Harrison will receive the Lewis S. Rosenstiel Award for Distinguished Work in Basic Medical Research. He will deliver a public lecture on his accomplishments followed by a ceremony in his honor. Harrison, the Giovanni Armenise-Harvard Professor of Basic Medical Sciences, was recognized for his fundamental and far-reaching studies of protein structure using X-ray crystallography.

**March 13, 2019.** Without Rosalind Franklin's knowledge, Maurice Wilkins shared her unpublished work with Crick and Watson, including the ground breaking "Photo 51" that

The Wizard Cryo line of random sparse matrix screens is designed for scientists who want to avoid the additional step of optimizing a cryoprotectant condition. Every Wizard Cryo formulation flash-freezes to a clear, amorphous glass in liquid nitrogen or in a cryo-stream at 100K. Crystals can be frozen directly from their growth drops, avoiding the additional step of pre-equilibration with an artificial cryo-condition that can damage the crystal. Eleven different cryocrystallants and sparing use of glycerol ensures a broad sampling of possible cryo conditions. Choose from Wizard Cryo 1 or 2 formulations in tubes or Wizard Cryo 1 and 2 together in a 96-well matrix block.

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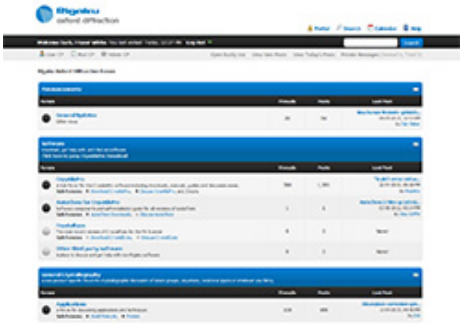
**Rigaku Oxford Diffraction Forum**



**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.

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**Survey of the Month**

captured DNA's double-helix structure. The three men created a model using Franklin's photo and, a decade later, they received Nobel Prizes for the discovery. The Nora Theatre Company, based at Central Square Theater in Cambridge, MA, produced a play based on that true story — titled "Photograph 51" — this season as our world grapples with #MeToo and gender inequity with greater intensity.

**March 14, 2019.** Barbara Low was a pioneer in X-ray crystallography. Her early work in the 1940s helped reveal the shape of the penicillin molecule, the world's first antibiotic, and helped usher in the age of antibiotics. Low joined the faculty of the Columbia University Vagelos College of Physicians and Surgeons in 1956. She died on Jan. 10 at her home in the Riverdale section of the Bronx. She was 98.

**March 15, 2019.** One of carbon monoxide's distinguishing features is a two-way bonding motif to metals, in which CO donates electrons to the metal while the metal simultaneously engages in "back bonding" in the other direction. Theory has suggested that the isoelectronic boron fluoride diatomic, BF, would be even more effective at both types of bonding. Myles Drance et al. at UCSD report synthesis of a terminal iron-BF complex, with donor and acceptor characteristics that compare favorably to analogous CO and $N_2$ complexes.

**March 15, 2019.** X-ray crystallography has revealed the existence of a double helical structure in a synthetic macromolecule known for thirty years. The discovery could open up novel applications for the high-strength polymer, called PBDT [poly(2,2'-disulfonyl-4,4'-benzidine terephthalamide)], beyond the original electrochemical and battery applications, for which it has been investigated recently.

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## Product Spotlight

**XtaLAB Synergy-DW**

One source with two high-flux wavelengths is the foundation of the revolutionary XtaLAB Synergy-DW single crystal X-ray diffractometer. It combines the increased flux of a rotating anode X-ray source with the flexibility of two different wavelengths, making it ideal for laboratories exploring a wide range of research interests.

**Configuration**

The XtaLAB Synergy-DW diffractometer is based on the proven, low-maintenance MicroMax-007 HF microfocus rotating anode. The target is constructed with two different X-ray source materials (Cu and Mo) and is coupled with an auto-switching dual wavelength optic. Copper or molybdenum X-ray radiation is available at the click of a button. The XtaLAB Synergy-DW offers up to 12x higher flux compared to the standard sealed tube X-ray sources and, utilizing only one generator, means overall maintenance is reduced.

Rounding out the XtaLAB Synergy-DW configuration is the fast and efficient four-circle kappa goniometer which is compatible with a wide range of detectors including the HyPix-6000HE and other Hybrid Photon Counting (HPC) X-ray detectors e.g. PILATUS and EIGER detectors.


**March 2019 SCX Survey**

**Let us test our ability to prognosticate. This edition of Crystallography Times is scheduled to post a couple of days before March 29, the deadline for Brexit.**

**The UK will:**

- Leave EU w/ agreement
- Leave EU w/o an agreement
- Ask for an extension
- Ask to stay in the EU

**Take the Survey**

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**Last Month's Survey**

In the February 11 issue of *Nature*, C. K. Gunsalus, Marcia K. McNutt, Brian C. Martinson, Larry R. Faulkner & Robert M. Nerem call for a US advisory board on research integrity.

Is it time for such a board to "to ensure safety, efficiency, and integrity while facilitating scientific progress and the optimal use of researchers' time"?

**Features**

- Access to two wavelengths in one compact system
- 12x higher flux than sealed tube X-ray sources
- Low maintenance, high performance system
- Uses CrysAlis$^{Pro}$ software with both PX and SMX modes

**Benefits**

- Multi-functional diffractometer to cover you wherever your research takes you
- High flux performance means you all your crystallography needs can be carried out 'in-house'
- Very little downtime and easy maintenance
- No need to purchase extra software for different applications

***For more information, watch our video on the XtaLAB Synergy-DW***

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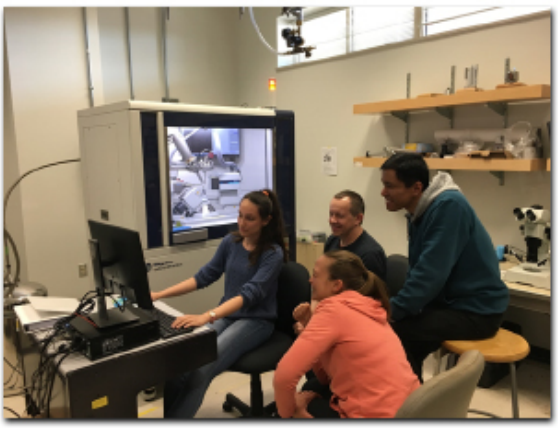
## Lab in the Spotlight

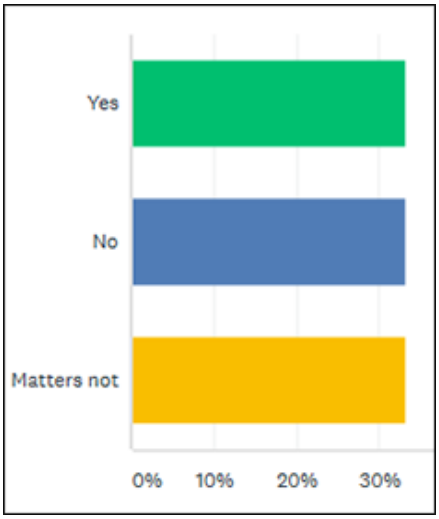
**Shatruk Group**

The group of Michael Shatruk at the Department of Chemistry and Biochemistry at Florida State University in Tallahassee works in a broadly defined area of advanced functional materials. Specific research interests include photo-switchable molecular materials, intermetallic magnets for magnetic refrigeration and electric vehicles, and low-dimensional magnetic materials such as spin-frustrated 2D magnets and nanomagnets. The disciplinary focus of the group's work lies within inorganic materials chemistry, with a strong interdisciplinary crossover to physical and organic chemistry, as well as to condensed matter physics and machine learning. The students and postdocs obtain diverse training in inorganic and organic syntheses, X-ray and neutron scattering methods, magnetic and electrical property measurements, optical, infrared, NMR, and EPR spectroscopy, as well as computational approaches to elucidation and discovery of new functional materials.

A Rigaku Oxford Diffraction Synergy-S was recently installed at FSU, with the funding support from the NSF-MRI program. The Shatruk group has been actively using the new diffractometer to determine structures of the aforementioned novel materials. Other users include Professors Igor Alabugin, Naresh Dalal, James Frederich, Susan Latturner and Biwu Ma, and Professor Emeritus Ron Clark.



Left to right: Ökten, Judy, Mike, and Xinsong setting up a 0.45 Å data collection on a novel Fe-TCNQ sample. Note the smiles on everyone's face.




**Videos of the Month**

Lady Gaga's Academy Award for Best Original Song reminded me of this hilarious parody of Bad Romance filmed here at the Texas Medical Center. In case you missed it the first time, here it is again:

Watch the Video

**Subscribe to Rigaku eNewsletters**


Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on X-ray crystallography.

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## Useful Link

**IUCr Online Dictionary of Crystallography (ODC)**

Here is a link to the IUCr Online Dictionary of Crystallography (ODC) maintained by the Commission for Crystallographic Nomenclature (CCN) of the International Union of Crystallography (IUCr). You will find hyperlinks from IUCr journal articles to terms defined here.

## Selected Recent Crystallographic Papers

**Steinberg's theorem for crystallographic complex reflection groups.** Puente, Philip; Shepler, Anne V. *Journal of Algebra*. Mar2019, Vol. 522, p332-350. 19p. DOI: 10.1016/j.jalgebra.2018.11.032.

**Convenient framework of poly functionalized (E)-2-benzylideno-(Z)-carbazolylideno cyanoacetamides via rearrangements as an efficient antibiofilm inhibitors with SAR study.** Sathiyachandran, Perumal; Jayamanoharan, Jabastin; Nesterov, Vladimir N.; Prasad, Karnam Jayarampillai Rajendra. *Bioorganic & Medicinal Chemistry*. Mar2019, Vol. 27 Issue 5, p777-784. 8p. DOI: 10.1016/j.bmc.2019.01.015.

**Synthesis, characterization and reactivity of non-heme 1st row transition metal-superoxo intermediates.** Noh, Hyeonju; Cho, Jaeheung. *Coordination Chemistry Reviews*. Mar2019, Vol. 382, p126-144. 19p. DOI: 10.1016/j.ccr.2018.12.006.

**Assembly of two hybrid organic-inorganic hexatantalate.** Ma, Yachun; Sun, Junjun; Li, Chen; Li, Nan; Ma, Pengtao; Zhang, Dongdi; Wang, Guan; Niu, Jingyang. *Inorganic Chemistry Communications*. Mar2019, Vol. 101, p6-10. 5p. DOI: 10.1016/j.inoche.2019.01.004.

**Synthesis and characterization of five diiron ethanedithiolate complexes with acetate group and phosphine ligands.** Chen, Fei-Yan; He, Jiao; Mu, Chao; Liu, Xu-Feng; Li, Yu-Long; Jiang, Zhong-Qing; Wu, Hong-Ke. *Polyhedron*. Mar2019, Vol. 160, p74-82. 9p. DOI: 10.1016/j.poly.2018.12.027.

**Substitution reactions of diiron diselenolato complex with bisphosphine ligands.** Li, Qian-Li; Lü, Shuang; Zhang, Ru-Fen; Zhao, Dong; Ma, Chun-Lin. *Polyhedron*. Mar2019, Vol. 160, p255-260. 6p. DOI: 10.1016/j.poly.2018.12.044.

**Evaluating the importance of fractional Z' polymorphs in a trifluoromethylated N,N'-diphenyloxalamide derivative.** Bhandary, Subhrajyoti; Panini, Piyush; Chopra, Deepak. *CrystEngComm*. 3/14/2019, Vol. 21 Issue 10, p1543-1547. 5p. DOI: 10.1039/c8ce02163e.

**Molecular insights into the mechanism of 4-hydroxyphenylpyruvate dioxygenase inhibition: enzyme kinetics, X-ray crystallography and computational simulations.** Lin, Hong-Yan; Yang, Jing-Fang; Wang, Da-Wei; Hao, Ge-Fei; Dong, Jiang-Qing; Wang, Yu-Xia; Yang, Wen-Chao; Wu, Jia-Wei; Zhan, Chang-Guo; Yang, Guang-Fu. *FEBS Journal*. Mar2019, Vol. 286 Issue 5, p975-990. 16p. DOI: 10.1111/febs.14747.

**Pnictogen ligand coordination to an iron-sulfur compound.** Donovan, Elizabeth S.; Plummer, Hannah M.; Parada, Alberto Sosa; Nichol, Gary S.; Felton, Greg A.N. *Inorganica Chimica Acta*. Mar2019, Vol. 487, p387-394. 8p. DOI: 10.1016/j.ica.2018.12.035.

**Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure–activity studies.** Kumar, Prashant; Gruza, Barbara; Bojarowski, Slawomir Antoni; Dominiak, Paulina Maria. *Acta Crystallographica. Section A, Foundations & Advances*. Mar2019, Vol. 75 Issue 2, p398-408. 11p. DOI: 10.1107/S2053273319000482.

**Finite groups of the same type as suzuki groups.** Alavi, Seyed Hassan; Daneshkhah, Ashraf; Mosaed, Hosein Parvizi. *International Journal of Group Theory*. 2019, Vol. 8 Issue 1, p35-42. 8p. DOI: 10.22108/ijgt.2017.21556.

**Synthesis, X-ray structures and biological properties of palladium(II) complexes of 1,2-dimethylimidazole and benzimidazole.** Sadaf, Haseeba; Imtiaz-ud-Din; Zahra, Syeda Saniya; Ihsan-ul-Haq; Nadeem, Shafqat; Tahir, Muhammad Nawaz; Ahmad, Saeed; Andleeb, Sohaila. *Polyhedron*. Mar2019, Vol. 160, p101-107. 7p. DOI: 10.1016/j.poly.2018.12.021.

**Crystal Structure of CC Chemokine Receptor 2A in Complex with an Orthosteric**

**Antagonist Provides Insights for the Design of Selective Antagonists.** Apel, Anna-Katharina; Cheng, Robert K.Y.; Tautermann, Christofer S.; Brauchle, Michael; Huang, Chia-Ying; Pautsch, Alexander; Hennig, Michael; Nar, Herbert; Schnapp, Gisela. *Structure*. Mar2019, Vol. 27 Issue 3, p427-427. 1p. DOI: 10.1016/j.str.2018.10.027.

**Iridium(I) homobinuclear complexes containing salen-type ligands as bridge.** Alvarado-Monzón, José C.; López, Jorge A.; de Riquer, Gabriel A. Andreu; Cristobal, Crispin; Flores-Alamo, Marcos; Ruiz-Azuara, Lena. *Polyhedron*. Mar2019, Vol. 161, p243-250. 8p. DOI: 10.1016/j.poly.2019.01.022.

**Structural, thermal and magnetic investigations of cobalt ferrite doped with $Zn^{2+}$ and $Cd^{2+}$ synthesized by auto combustion method.** Kaur, Harpreet; Singh, Amrik; Kumar, Vijay; Ahlawat, Dharamvir Singh. Journal of Magnetism & Magnetic Materials. Mar2019, Vol. 474, p505-511. 7p. DOI: 10.1016/j.jmmm.2018.11.010.

**Synthesis, characterization and biological evaluation of Zn(II) and Co(II) complexes of N-allylimidazole as potential hypoxia-targeting agents.** Parshina, Lidiya N.; Grishchenko, Lyudmila A.; Smirnov, Vladimir I.; Borodina, Tat'yana N.; Shakhmardanova, Svetlana A.; Tarasov, Vadim V.; Apartsin, Konstantin A.; Kireeva, Victoria V.; Trofimov, Boris A. *Polyhedron*. Mar2019, Vol. 161, p126-131. 6p. DOI: 10.1016/j.poly.2019.01.005.

**Zinc(II) and cadmium(II) halide complexes with caffeine: Synthesis, X-ray crystal structure, cytotoxicity and genotoxicity studies.** Rukk, Nataliya S.; Kuzmina, Lyudmila G.; Shamsiev, Ravshan S.; Davydova, Galina A.; Mironova, Elena A.; Ermakov, Artem M.; Buzanov, Grigory A.; Skryabina, Alena Yu.; Streletskii, Andrej N.; Vorob'eva, Galina A.; Retivov, Vasilii M.; Volkov, Pavel A.; Belus, Svetlana K.; Kozhukhova, Evgeniya I.; Krasnoperova, Valeriya N. *Inorganica Chimica Acta*. Mar2019, Vol. 487, p184-200. 17p. DOI: 10.1016/j.ica.2018.11.036.

**Structure of the UHRF1 Tandem Tudor Domain Bound to a Methylated Non-histone Protein, LIG1, Reveals Rules for Binding and Regulation.** Kori, Satomi; Ferry, Laure; Matano, Shohei; Jimenji, Tomohiro; Kodera, Noriyuki; Tsusaka, Takeshi; Matsumura, Rumie; Oda, Takashi; Sato, Mamoru; Dohmae, Naoshi; Ando, Toshio; Shinkai, Yoichi; Defossez, Pierre-Antoine; Arita, Kyohei. *Structure*. Mar2019, Vol. 27 Issue 3, p485-485. 1p. DOI: 10.1016/j.str.2018.11.012.

**Affinity Improvement of a Cancer-Targeted Antibody through Alanine-Induced Adjustment of Antigen-Antibody Interface.** Yamashita, Takefumi; Mizohata, Eiichi; Nagatoishi, Satoru; Watanabe, Takahiro; Nakakido, Makoto; Iwanari, Hiroko; Mochizuki, Yasuhiro; Nakayama, Taisuke; Kado, Yuji; Yokota, Yuki; Matsumura, Hiroyoshi; Kawamura, Takeshi; Kodama, Tatsuhiko; Hamakubo, Takao; Inoue, Tsuyoshi; Fujitani, Hideaki; Tsumoto, Kouhei. *Structure*. Mar2019, Vol. 27 Issue 3, p519-519. 1p. DOI: 10.1016/j.str.2018.11.002.

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## Book Review


***Freedom's Laboratory: The Cold War Struggle for the Soul of Science***
**By Audra J. Wolfe**
**ISBN 9781421426730**

*Freedom's Laboratory* provides a detailed history of science and its role in society during the Cold War. Wolfe takes a deep dive into the role the United States government played in scientific inquiry and discovery around the world in the years following World War II. The Space Race was merely one facet of the heightened, science-related tensions between the capitalist United States and the communist Soviet Union.

Wolfe begins by introducing the concept of scientific freedom: the idea that science is an apolitical subject—or at least should be—which, ironically, is a notion fundamentally fueled by the powers that be. In other words, the ideology of scientific freedom was in many ways created by the United States government during the Cold War, and perpetuated both in America and around the world via public propaganda and covert CIA operations. Scientific freedom, like truth in history, seems to be a matter of perspective.

Despite the escalation of tensions between the ideology of scientific freedom and communism during the Cold War, the disconnect existed even before America entered World War II. JD Bernal, the well-known British crystallographer, published a book called *The Social Function of Science* in 1939. Bernal criticized the role of American capitalism in curtailing scientific discovery, and proposed that the Soviet approach was the best means of bettering society through scientific advancement. Although Bernal's book sparked intense academic debate at the time of its publication, it provided a crystallized version of an argument that had been circulating in academia for decades, since the revolution that

transformed Russia from an imperial monarchy to a communist country.

Starting with Bernal's book, Wolfe weaves an intricate and often hard-to-follow historical narrative—though that is less of a statement about Wolfe's talent as an author and more to do with the subject matter. The history of scientific freedom during the Cold War is convoluted, with innumerable players both on the world stage and behind the scenes, from scientists to politicians to world leaders to covert operatives. Wolfe's dedication to providing a balanced history, both comprehensive and concise, is decidedly admirable.

It's a complicated concept, to consider that the very ideal of scientific freedom that defines American research was contrived and carefully cultivated by our government. Wolfe plays the role of neutral historian, presenting a series of factual events and letting readers draw their own conclusions, at least until the epilogue.

Wolfe saves the best (or worst, depending on how you look at it) for last, comparing the tensions between society and science in the 1950s and 1960s to those that exist today. It is hard to ignore the glaring parallels between international tensions over fifty years ago and those occurring now—and disorienting to watch the repetition of history unfolding in one's own lifetime.

In the wake of the open-mindedness and supportiveness of the Obama administration, the Trump administration has taken a sharply different tack regarding the relationship between science and the government. Only a few months after our current president took office, scientists across the country gathered in Washington, DC for the March for Science—something Wolfe discusses in her epilogue. It is worth considering the implications of living in a society where political demonstrations are not only geared towards basic human rights and equality, but the critical importance of freedom in scientific discovery.

Science, fundamentally, should be a pursuit of fact as proven by rigorous experimentation and results, whereas truth in this time seems to be a relative concept dependent on perspective and feeling. Given the current administration's adamant disregard for fact, or rather, its constant declaration of fiction as truth, it is not hard to understand why science itself—the pursuit of evidence-based fact—is considered a threat.

Review by Jeanette S. Ferrara, MA


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